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- Bertault, M., see J. Sworakowski 220 (1994) 197
- Besenbacher, F., see M. Foss 215 (1993) 535
- Bethune, D.S., see C.-H. Park 213 (1993) 196
- Bezel, I.V., S.V. Chekalin, Yu.A. Matveets, A.G. Stepanov, A.P. Yartsev and V.S. Letokhov, Two-photon absorption of powerful femtosecond pulses in  $\text{C}_{60}$  film 218 (1994) 475
- Bhat, S.G.T., see R.V. Jasra 211 (1993) 214
- Bhattacharyya, K., see N. Sarkar 218 (1994) 492
- Bhattacharyya, S.P., see P. Dutta 212 (1993) 677
- Bi, X., see Y. Wang 217 (1994) 413
- Bi, X.-X., see Y. Wang 211 (1993) 341
- Bi, X.-X., see J.M. Holden 220 (1994) 186
- Bierl, R., see S. Schneider 219 (1994) 433
- Biermann, M., see M. Neeb 212 (1993) 205
- Bieze, T.W.N., J.R.C. van der Maarel and J.C. Leyte, The intramolecular OH bond length of water in a concentrated poly(ethyleneoxide) solution. An NMR relaxation study 216 (1993) 56
- Bigot, B., see S.A. Borshch 212 (1993) 398
- Bill, H., see C. Pédrini 220 (1994) 433
- Billing, G.D. and R.E. Kolesnick, Semi-classical calculations of rate constants for vibrational transitions in hydrogen 215 (1993) 571
- Billing, G.D., see L. Goubert 219 (1994) 360
- Bintz, K.L., D.L. Thompson, K.L. Kompa and R.D. Levine, The direct overtone pumping of polyatomic molecules 215 (1993) 455
- Bird, D.M., L.J. Clarke, M.C. Payne and I. Stich, Dissociation of  $\text{H}_2$  on  $\text{Mg}(0001)$  212 (1993) 518
- Bird, D.M., see J.A. White 213 (1993) 422
- Bishop, D.M. and S.M. Cybulski, Calculation of electromagnetic properties of the noble gases 211 (1993) 255
- Bisht, P.B., H. Petek and K. Yoshihara, Exciplex formation in van der Waals complexes of naphthalene-triethylamine in a supersonic jet 213 (1993) 75
- Bist, H.D., see R.K. Singh 213 (1993) 210
- Bittl, R., see A. Van der Est 212 (1993) 561
- Bittl, R., Matrix elements of spin operators in exchange coupled tetrameric metal clusters 215 (1993) 279
- Blain, M., see L. Koubi 217 (1994) 544
- Blake, G.A., see P.A. Stockman 212 (1993) 298
- Blasberg, T. and D. Suter, Nuclear spin relaxation of  $\text{Pr}^{3+}$  in  $\text{YAlO}_3$ . A temperature-dependent optical-rf double-resonance study 215 (1993) 668
- Blasse, G., G.J. Dirksen, P. Zhiwu, G. Wehrum and R. Hoppe, Luminescence and energy migration in  $\text{Ba}_3\text{NaNbO}_6$  and  $\text{Ba}_3\text{NaTaO}_6$  215 (1993) 363



- Blasse, G., see E. Bayer 216 (1993) 228
- Blau, W.J., see P. Lemoine 220 (1994) 177
- Blechta, V. and R. Freeman, Multi-site Hadamard NMR spectroscopy 215 (1993) 341
- Blonski, S. and S.H. Garofalini, Molecular dynamics simulations of  $\gamma$ -alumina surface stabilization by deposited silicon ions 211 (1993) 575
- Bludau, H., M. Gierer, H. Over and G. Ertl, A low-energy electron diffraction analysis of the  $(\sqrt{3} \times \sqrt{3})R30^\circ$  structure of molecular nitrogen adsorbed on Ru(0001) 219 (1994) 452
- Bludský, O., see R. Kobayashi 215 (1993) 576
- Bo, C., see C. Sousa 215 (1993) 97
- Bodenhausen, G., see S. Nicula 219 (1994) 291
- Bodesheim, M., see R. Schmidt 213 (1993) 111
- Bolender, J.P., D.H. Metcalf and F.S. Richardson, Chirality-dependent intermolecular interactions probed by time-resolved chiroptical luminescence measurements of enantio-differential excited-state quenching kinetics 213 (1993) 131
- Bollati, R.A. and J.C. Ferrero, Quasiclassical trajectory calculations of the transition probability function in the vibrational relaxation of HgBr( $B^2\Sigma, v=52$ ) by monoatomic gases 218 (1994) 159
- Bonačić-Koutecký, V., P. Fantucci, C. Fuchs, C. Gatti, J. Pittner and S. Polezzo, Ab initio predictions of optically allowed transitions in Na<sub>20</sub>. Nature of excitations and influence of geometry 213 (1993) 522
- Bond, P., P.N., J. Fletcher, P.A. Gorry and M.E. Pemble, Reactive scattering of Cl<sub>2</sub> on GaAs (100). Cl<sub>2</sub> and GaCl product distributions (Chem. Phys. Lett. 208 (1993) 269). Erratum 211 (1993) 649
- Bondybey, V.E., see N. Caspary 212 (1993) 329
- Bondybey, V.E., see M. Fárník 216 (1993) 458
- Bondybey, V.E., see C. Berg 216 (1993) 465
- Bondybey, V.E., see G. Schallmoser 219 (1994) 101
- Bonneau, M., see S. Douin 216 (1993) 215
- Bonnet, L., J.C. Rayez and P. Halvick, A geometric model for the regular dynamical behaviour of collinear three-atom reactions involving an intermediate well 216 (1993) 11
- Bonosi, F., see G. Ricciardi 215 (1993) 541
- Bonser, D., see L.A. Keeling 217 (1994) 136
- Boo, D.W. and Y.T. Lee, Infrared spectra of CH<sub>5</sub><sup>+</sup> core in CH<sub>5</sub><sup>+</sup>(H<sub>2</sub>) 211 (1993) 358
- Boogaarts, M.G.H., see G. Meijer 217 (1994) 112
- Booth, C., see C.-H. Park 213 (1993) 196
- Booze, J.A., see D.E. Govoni 216 (1993) 525
- Boraas, K., see Z. Lin 217 (1994) 239
- Borg, R.A.J., E.R. Waclawik, Mudjijono and W.D. Lawrance, A strong collision partner dependence for vibrational energy transfer in benzene and benzene-*d*<sub>6</sub>. He versus D<sub>2</sub> 218 (1994) 320
- Borrás-Almenar, J.J., E. Coronado, H.M. Kishinevsky and B.S. Tsukerblat, Semiclassical approximation in the magnetic problem of exchange-coupled mixed valence clusters 217 (1994) 525
- Borrmann, A., see L.M. Finney 214 (1993) 159
- Borrmann, A., see Z. Li 214 (1993) 362
- Borshch, S.A. and B. Bigot, Magnetic properties of the mixed-valence heteropoly blues with a Keggin structure 212 (1993) 398
- Borzsák, I. and A. Baranyai, The overlap volume in hard spheres under shear 216 (1993) 329
- Botella, V., O. Castaño, P. Fernández-Serra and Y.G. Smeyers, Multiple solutions and spatial symmetry properties of singlet and triplet states in the half-projected Hartree-Fock method 219 (1994) 497



- Botschwina, P., M. Oswald, J. Flügge, Ä. Heyl and R. Oswald, Ab initio spectroscopic constants and the equilibrium geometry of HCCF (Chem. Phys. Letters 209 (1993) 117).  
Erratum 215 (1993) 681
- Boulon, G., see J.A. Mares 217 (1994) 105
- Boustani, I., see H.-P. Liebermann 214 (1993) 381
- Boutin, A., see F.M. Bénérière 215 (1993) 301
- Boutin, A., B. Rousseau and A.H. Fuchs, The temperature-size phase diagram of large SF<sub>6</sub> clusters by computer simulation 218 (1994) 122
- Boutin, A., R.J.-M. Pellenq and D. Nicholson, Molecular simulation of the stepped adsorption isotherm of methane in AlPO<sub>4</sub>-5 219 (1994) 484
- Bouttet, D., see C. Pédrini 220 (1994) 433
- Bowers, M.T., see G. von Helden 212 (1993) 241, 247
- Bowman, J.M., A test of an adiabatic treatment of rotation for vibration/rotation energies of polyatomic molecules 217 (1994) 36
- Boyd, R.J., see L.A. Eriksson 211 (1993) 88
- Boyd, R.J., see J. Kong 217 (1994) 24
- Brabec, C.J., A. Maiti and J. Bernholc, Structural defects and the shape of large fullerenes 219 (1994) 473
- Bradley, A., see J.S. Francisco 214 (1993) 77
- Bradshaw, A.M., see M. Neeb 212 (1993) 205
- Bradshaw, A.M., see B. Rausenberger 215 (1993) 109
- Bradshaw, A.M., see M. Ondřejček 215 (1993) 528
- Braga, M. and S. Larsson, Correlation and relaxation effects in the electronic coupling between acetylenic  $\pi$  and  $\pi^*$  electrons through saturated and aromatic spacers 213 (1993) 217
- Bramble, S.K., see J. Baker 213 (1993) 297
- Brand, H.R., see M. Diewald 216 (1993) 566
- Brandl, V., see O. Dippel 216 (1993) 418
- Braun, C.L., see S.N. Smirnov 217 (1994) 167
- Braune, M. and H. Engel, Compound rotation of spiral waves in active media with periodically modulated excitability 211 (1993) 534
- Bravic, G., see M. Lequan 213 (1993) 71
- Bréchignac, P., see S. Douin 216 (1993) 215
- Brédas, J.L., see M. Fahlman 214 (1993) 327
- Brédas, J.L. and A.J. Heeger, Influence of donor and acceptor substituents on the electronic characteristics of poly(paraphenylene vinylene) and poly(paraphenylene) 217 (1994) 507
- Breest, A., see S. Grimme 213 (1993) 32
- Breheret, E., see F. Lahmani 220 (1994) 235
- Breidohr, R., O. Shestakov and E.H. Fink, The  $a^3\Sigma_u^+ (a_11_u) \rightarrow X^1\Sigma_g^+ (X0_g^+)$  transition of Sb<sub>2</sub> 218 (1994) 13
- Brendsdal, E., see I. Gutman 219 (1994) 355
- Brenier, A., see J.A. Mares 217 (1994) 105
- Brenner, L.J., J. Senekowitsch and R.E. Wyatt, Coupled cluster calculation of the in-plane harmonic force field of benzene 215 (1993) 63
- Breton, J. and E. Navedryk, S<sub>0</sub>→T<sub>1</sub> infrared difference spectrum of the triplet state of the primary electron donor in *Rb. sphaeroides* photosynthetic bacterial reaction centers 213 (1993) 571
- Bridges, F., see C.-H. Park 213 (1993) 196
- Brier, P.N., see P. Bond 211 (1993) 649
- Brillante, A., M. Cau, R.G. Della Valle and E. Venuti, The effect of pressure on the photo-dimerization of 7-methoxycoumarin crystal 218 (1994) 568

- Brink, C., see L.H. Andersen 217 (1994) 204
- Brion, J., A. Chakir, D. Daumont, J. Malicet and C. Parisse, High-resolution laboratory absorption cross section of  $O_3$ . Temperature effect 213 (1993) 610
- Brocklehurst, B., Radio-luminescence of alkane solutions. Comparison of experiment and simulation over a wide energy range 211 (1993) 31
- Bronnikov, D.K., see A.E. Wiskerke 216 (1993) 93
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- Broyer, M., see K. Kobe 213 (1993) 554
- Broyer, M., see M. Pellarin 217 (1994) 349
- Brugmans, M.J.P., A.W. Kleyn, A. Lagendijk, W.P.J.H. Jacobs and R.A. van Santen, Hydrogen bonding in acidic zeolites observed by time-resolved vibrational spectroscopy 217 (1994) 117
- Brühwiler, P.A., S. Andersson, M. Dippel, N. Mårtensson, P.A. Demirev and B.U.R. Sundqvist, Hydrogenation of solid  $C_{60}$  by atomic hydrogen 214 (1993) 45
- Brunvoll, J., see I. Gutman 219 (1994) 355
- Brusa, R.S., see G. Karwasz 211 (1993) 529
- Buchachenko, A.A., A.Yu. Baisogolov and N.F. Stepanov, The vibrational predissociation lifetime of the  $He...N_2^+(X, v=1)$  complex 220 (1994) 93
- Büchel, M., see Z. Sekkat 220 (1994) 497
- Buchen, Th. and P. Güthlich, Thermal and light-induced spin crossover in iron(II) complexes with monodentate tetrazole ligands carrying long alkyl chains in the 1-position 220 (1994) 262
- Buckingham, A.D. and R.M. Olegário, Hyperfine coupling in alkaline earth monofluorides. Limitations of the ionic model 212 (1993) 253
- Buenker, R.J., see Y. Li 212 (1993) 185
- Buenker, R.J., see H.-P. Liebermann 214 (1993) 381
- Bulanin, M.O., Spectral interpretation of the refractivity and dielectric virial coefficients of atomic gases 217 (1994) 466
- Bungay, A.R., S.V. Popov, Yu.P. Svirko and N.I. Zheludev, Time-non-invariant linear birefringence and dichroism due to spin-orbit interaction 217 (1994) 249
- Buntine, M.A., D.J. Lavrich, C.E. Dessent, M.G. Scarton and M.A. Johnson, Photoinitiation of the  $O^- + H_2O \rightarrow OH^- + OH$  ion-molecule reaction within the  $O_2^- \cdot H_2O$  binary complex 216 (1993) 471
- Burba, M.E., see S.K. Lim 216 (1993) 405
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- Burshtein, Z., see R. Gvishi 212 (1993) 463; 213 (1993) 338
- Burt, J.A. and G.A. Crosby, Barriers to energy migration in mixed-ligand zinc(II) complexes 220 (1994) 493
- Burton, N.A., see R.J. Hall 220 (1994) 129
- Butler, D.A., B.E. Hayden and J.D. Jones, Precursor dynamics in dissociative hydrogen adsorption on W(100) 217 (1994) 423
- Buttet, J., see S. Fedrigo 211 (1993) 166
- Byrne, H.J., see L. Akselrod 212 (1993) 384; 215 (1993) 131

- Caballol, R., see À. Povill 218 (1994) 283
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- Cahill, P.A., see C.C. Henderson 213 (1993) 383
- Cai, Z.-L., X.-G. Zhang and X.-Y. Wang, Ab initio study of four low-lying electronic states of the CCS molecule 213 (1993) 168
- Cai, Z.-L. and J.-L. Bai, Ab initio study of the electronic spectrum of the SF<sub>2</sub> radical 220 (1994) 109
- Caldino G., U., M. Voda, F. Jaque, J. García Solé and A.A. Kaminskii, Nd<sup>3+</sup> multisites in the disordered Ca<sub>3</sub>Ga<sub>2</sub>Ge<sub>3</sub>O<sub>12</sub> laser crystal 213 (1993) 84
- Caldwell, C.D., see S.J. Schaphorst 213 (1993) 315
- Calvo Hernández, A., see J.M.M. Roco 216 (1993) 593
- Campargue, A., see A. Charvát 214 (1993) 495
- Canet, D., J.B. Robert and P. Tekely, <sup>13</sup>C NMR relaxation time of fullerene as a function of magnetic field 212 (1993) 483
- Cao, D., see Y. Chen 211 (1993) 449
- Capitelli, M., see G. Colonna 213 (1993) 5
- Carlson, M., see G. Sundström 218 (1994) 17
- Carnell, M. and S.D. Peyerimhoff, Assignment of the vacuum-ultraviolet spectrum of ethylene sulphide 212 (1993) 654
- Carrasquillo M., E., see J.S. Baskin 214 (1993) 257
- Carrasquillo M., E., see R. Huang 216 (1993) 108, 115
- Carrington, A., C.A. Leach, A.J. Marr, C.H. Pyne, A.M. Shaw, M.R. Viant and Y.D. West, Near-dissociation microwave spectra of rare-gas diatomic ions 212 (1993) 473
- Carruthers, J.R., see J.D. Gale 216 (1993) 155
- Carter, E.A., see B. Hartke 216 (1993) 324
- Cartier, S.F., B.D. May, B.J. Toleno, J. Purnell, S. Wei and A.W. Castleman Jr., The production of metallocarbohedrenes by the direct laser vaporization of the carbides of titanium and zirconium 220 (1994) 23
- Cartland, H.E., see B.M. Rice 211 (1993) 283
- Casavecchia, P., see N. Balucani 211 (1993) 469
- Caselli, M., F. Momicchioli and G. Ponterini, Modelling of the cis–trans partitioning in the photoisomerizations of cyanines and stilbene derivatives 216 (1993) 41
- Caspar, J.V. and Y. Wang, Excited state electron transfer of fullerenes. Singlet states versus triplet states 218 (1994) 221
- Caspary, N., B.E. Wurfel, A. Thoma, G. Schallmoser and V.E. Bondybey, Infrared identification of the FCS radical in an argon matrix 212 (1993) 329
- Cassidei, L., see G. Petrella 212 (1993) 512
- Castanheira, E.M.S., see A.T. Reis e Sousa 213 (1993) 333
- Castano, O., see V. Botella 219 (1994) 497
- Casties, A., see J. Mai 211 (1993) 197
- Castillejo, M., J.M. Figuera, H.A. Zeaiter and M. Oujja, Rate constants for removal by noble gases of selected rotational levels of methylene <sup>1</sup>B<sub>1</sub>(0, 14, 0) 214 (1993) 227
- Castleman Jr., A.W., see S.F. Cartier 220 (1994) 23
- Castleman Jr., A.W., see Z. Shi 220 (1994) 274
- Catlow, C.R.A., see J.D. Gale 216 (1993) 155
- Cau, M., see A. Brillante 218 (1994) 568
- Caubet, P. and G. Dorthé, Origin of C<sub>2</sub> high-pressure bands observed in the products of a microwave discharge through CO 218 (1994) 529



- Causà, M. and A. Zupan, Density functional LCAO calculation of periodic systems. A posteriori correction of the Hartree-Fock energy of covalent and ionic crystals 220 (1994) 145
- Cazzini, K., see P. Lemoine 220 (1994) 177
- Cazzoli, G., see C. Degli Esposti 214 (1993) 531
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- Cemic, F., see K.W. Kolasinski 219 (1994) 113
- Céolin, R., see B. Keita 215 (1993) 125
- Ceulemans, A. and G. Mys, The vector particle of tensor surface harmonic theory 219 (1994) 274
- Cháb, V., see M. Ondřejček 215 (1993) 528
- Chabach, D., see T.-H. Tran-Thi 213 (1993) 139
- Chabalowski, C.F., see B.M. Rice 211 (1993) 283
- Chakir, A., see J. Brion 213 (1993) 610
- Chakrabarti, A., S. Yashonath and C.N.R. Rao, Orientational glassy phases of  $C_{60}$  and neopentane. A Monte Carlo study 215 (1993) 591
- Chakravorty, S.J., see E.R. Davidson 217 (1994) 48
- Chambaud, G., see A. Spielfiedel 216 (1993) 162
- Chambers, C.C. and D.L. Thompson, Enhancement of vibrational mode mixing due to isomerization barrier crossings 218 (1994) 166
- Champagne, B. and Y. Öhrn, Ab initio longitudinal polarizabilities of conjugated stereoregular polymers with a carbon backbone 217 (1994) 551
- Chan, I.Y., C.M. Wong and D. Stehlik, Pressure dependence of the low-temperature tunneling rate for the hydrogen transfer in acridine-doped fluorene crystals 219 (1994) 187
- Chan, M.-C., see B. Fain 216 (1993) 551
- Chandler, C., see W. Zhu 217 (1994) 73
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- Chang, S.-H., see R.C. Haddon 218 (1994) 100
- Chang, T.-C., H.-W. Li, T.-C. Hsieh and S.-H. Chou, Picosecond time-resolved CSRS study of vibrational dephasing of bulk modes perturbed by electronic state of dilute impurities 213 (1993) 564
- Chang, T.C., see B. Fain 216 (1993) 551
- Chao, M., see P.-T. Chou 220 (1994) 229
- Charra, F., see J.-M. Nunzi 215 (1993) 114; 219 (1994) 349
- Charvát, A., A.A. Kachanov, A. Campargue, D. Permogorov and F. Stoeckel, High sensitivity intracavity absorption spectroscopy of  $CHD_3$  in the near infrared with a titanium:sapphire laser 214 (1993) 495
- Chasseau, D., see M. Lequan 213 (1993) 71
- Châtelain, A., see W.S. Bacsa 211 (1993) 346
- Chattaraj, P.K., S. Nath and A.B. Sannigrahi, Ab initio SCF study of maximum hardness and maximum molecular valency principles 212 (1993) 223
- Chattaraj, P.K. and S. Nath, Hardness dynamics in a chemical reaction 217 (1994) 342
- Chaudhuri, J., see R. Debnath 217 (1994) 357
- Chavy, C., C. Joachim and A. Altibelli, Interpretation of STM images:  $C_{60}$  on the gold(110) surface 214 (1993) 569
- Chavy, C., C. Joachim and A. Altibelli, Interpretation of STM images:  $C_{60}$  on the gold(110) surface (Chem. Phys. Letters 214 (1993) 569). Erratum 219 (1994) 502



- Chekalin, S.V., see I.V. Bezel 218 (1994) 475
- Chemerisov, S.D., O.Ya. Grinberg, D.S. Tipikin, Ya.S. Lebedev, H. Kurreck and K. Möbius, Mechanically induced radical pair formation in porphyrin-quinone and related donor-acceptor mixtures. Unusual stability and zero-field splittings 218 (1994) 353
- Chemseddine, A., Fibrous and oriented quantum dots. Synthesis and characterization 216 (1993) 265
- Chen, C., see Y. Chen 211 (1993) 449
- Chen, C.-C., H. Chang and C.-S. Hsue, A highly accurate calculation for the electronic states of  $H_2^+$  in B-spline basis 217 (1994) 486
- Chen, C.H., see R.B. Jones 212 (1993) 451
- Chen, J. and P.J. Dagdigan, Spectrally resolved fluorescence in the HNF (DNF)  $\tilde{A}^2A'$ - $\tilde{X}^2A''$  band system 213 (1993) 586
- Chen, K. and C. Pei, Time-resolved intensity patterns of photofragments by laser sheet illumination and two-dimensional imaging techniques 217 (1994) 471
- Chen, L., see L.A. Keeling 217 (1994) 136
- Chen, X., see H. Wang 216 (1993) 537
- Chen, Y., C. Chen, X. Ma, S. Li, Y. Chu and D. Cao, Energy transfer reaction for CS with metastable CO(a) 211 (1993) 449
- Cheng, P.Y., see P. DeRose 220 (1994) 207
- Cheng, W.-D., J.-S. Huuqang and Q.-E. Zhang, Electronic structure of the ground state and calculated spectrum of low-lying excited states of  $Mo_3X_4(aq)_9^{4+}$  ( $X=O, S$ ) cluster ions 216 (1993) 353
- Chergui, M., R. Reininger, E. Morikawa and A. Tramer, Control by density effects of the Rydberg-valence configuration mixing in matrix isolated NO 216 (1993) 34
- Chergui, M. and N. Schwentner, Experimental evidence to Rydbergization of antibonding molecular orbitals 219 (1994) 237
- Chermette, H., see F. Rogemond 219 (1994) 228
- Chernia, Z. and D. Gill, Reversible self-assembly of fluorescent dimers of anthracene derivative adsorbed on laponite 212 (1993) 57
- Chernozatonskii, L.A., see E.G. Gal'pern 214 (1993) 345
- Chernozatonskii, L.A., see A.A. Kharlamov 219 (1994) 457
- Cheskis, S., see A.A. Iogansen 212 (1993) 604
- Cheung, J.L., A.S. Kwok, K.A. Juvan, D.H. Leach and R.K. Chang, Stimulated low-frequency emission from anisotropic molecules in microdroplets 213 (1993) 309
- Chevaleyre, J., see R.F. Barrow 214 (1993) 293
- Ching, K.C., see M. Lequan 213 (1993) 71
- Chistykov, A.L., see E.G. Gal'pern 214 (1993) 345
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- Chong, D.P., Local density calculations of static dielectric properties of  $CH_{4-n}Cl_n$ ,  $n=0-4$  217 (1994) 539
- Chong, D.P., Local density studies of diatomic AB molecules, A, B=C, N, O, F, Si, P, S, and Cl 220 (1994) 102
- Chorkendorff, I., see J. Hall 216 (1993) 413
- Chou, P.-T., W.C. Cooper, J.H. Clements, S.L. Studer and C.P. Chang, A comparative study. The photophysics of 2-phenylbenzoxazoles and 2-phenylbenzothiazoles 216 (1993) 300

- Chou, P.-T., M. Chao, J.H. Clements, M.L. Martinez and C.-P. Chang, Excited-state intramolecular proton transfer for N-substituted-3-hydroxypyridinones 220 (1994) 229
- Chou, S.-H., see T.-C. Chang 213 (1993) 564
- Choudary, N.V., see R.V. Jasra 211 (1993) 214
- Chowdhury, P.K., see Awadhesh Kumar 212 (1993) 103
- Chowdhury, P.K., K.V.S. Rama Rao and J.P. Mittal, Infrared multiphoton dissociation of acrolein. Time-resolved observation of CO ( $\nu=1$ ) IR emission at 4.7  $\mu\text{m}$  218 (1994) 60
- Christensen, O.B. and J.K. Nørskov, Modeling the potassium promotion of CO bonding to Ni(100) 214 (1993) 443
- Christmann, K., see R. Koch 220 (1994) 172
- Chronister, E.L., see R.A. Crowell 216 (1993) 293
- Chu, B., see Q. Ying 219 (1994) 214
- Chu, K., G.U. Nienhaus and R. Philipp, Structural heterogeneity in proteins at cryogenic temperatures. Cooling rate dependence 216 (1993) 275
- Chu, S.-I., see Y. Huang 211 (1993) 601
- Chu, Y., see Y. Chen 211 (1993) 449
- Chupka, W.A., see Y. Wang 214 (1993) 290
- Chvoj, Z., see M. Ondřejček 215 (1993) 528
- Ciesielski, W., see N.D. Kushch 215 (1993) 137
- Cimiraglia, R. and H.-J. Hofmann, Rotation and inversion states in thermal E/Z isomerization of aromatic azo compounds 217 (1994) 430
- Cioslowski, J., Heats of formation of higher fullerenes from ab initio Hartree-Fock and correlation energy functional calculations 216 (1993) 389
- Cioslowski, J. and A. Nanayakkara, A new robust algorithm for fully automated determination of attractor interaction lines in molecules 219 (1994) 151
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- Clough, S., A.J. Horsewill, A.M. Alsanoosi, M.J. Barlow and M.R. Johnson, The spectrum of rotating wavepackets of hindered methyl groups 211 (1993) 637
- Coat, Y.L., see R. Azria 220 (1994) 417
- Cockett, M.C.R., J.G. Goode, K.P. Lawley and R.J. Donovan, The spectroscopy of Rydberg excited iodine-argon van der Waals complexes 214 (1993) 27
- Codling, K., see D.M. Smith 216 (1993) 493
- Cohen, M. and T. Feldmann, The systematic derivation of realizations of generators of Lie algebras 218 (1994) 147
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- Colonna, F. and E.M. Evleth, Conformationally invariant modeling of atomic charges 212 (1993) 665
- Colonna, G., C. Gorse, M. Capitelli, R. Winkler and J. Wilhelm, The influence of electron-electron collisions on electron energy distribution functions in  $\text{N}_2$  post discharge 213 (1993) 5

- Columbia, M.R. and P.A. Thiel, The stabilization of formate on Pt(111) by coadsorbed atomic oxygen 220 (1994) 167
- Colwell, S.M. and N.C. Handy, The determination of magnetisabilities using density functional theory 217 (1994) 271
- Comelli, G., see D. Arvanitis 211 (1993) 53
- Comelli, G., see C. Comicioli 214 (1993) 438
- Comicioli, C., V.R. Dhanak, G. Comelli, C. Astaldi, K.C. Prince, R. Rosei, A. Atrei and E. Zanazzi, Structure of Rh{110}(1×2) and Rh{110}(2×2)p2mg-O surfaces 214 (1993) 438
- Cong, P., H.P. Deuel and J.D. Simon, Using optical coherence to measure the ultrafast electronic dephasing of large molecules in room-temperature liquids 212 (1993) 367
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- Corongiu, G. and E. Clementi, Liquid water: density of states spectra of solvated water molecules with specific coordination 214 (1993) 367
- Corval, A., see S. Astilean 219 (1994) 95
- Cory, D.G., F.H. Laukien and W.E. Maas, NMR spectroscopy with radial pulses. p- and n-type selection COSY 212 (1993) 487
- Cotts, R.M., see S. Miyajima 212 (1993) 277
- Coussan, S., N. Bakkas, A. Loutellier, J.P. Perchard and S. Racine, Infrared photoisomerization of the methanol cyclic trimer trapped in a nitrogen matrix 217 (1994) 123
- Couto, M.S., see X.-Y. Liu 220 (1994) 53
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- Cramer, C.J., F.J. Dulles, J.W. Storer and S.E. Worthington, Full valence complete active space SCF, multireference CI, and density functional calculations of <sup>1</sup>A<sub>1</sub>-<sup>3</sup>B<sub>1</sub> singlet-triplet gaps for the valence-isoelectronic series BH<sub>2</sub><sup>-</sup>, CH<sub>2</sub>, NH<sub>2</sub><sup>+</sup>, AlH<sub>2</sub><sup>-</sup>, SiH<sub>2</sub>, PH<sub>2</sub><sup>+</sup>, GaH<sub>2</sub><sup>-</sup>, GeH<sub>2</sub>, and AsH<sub>2</sub><sup>+</sup> 218 (1994) 387
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- Croci, M., H.-J. Müschenborn, F. Güttler, A. Renn and U.P. Wild, Single molecule spectroscopy: pressure effect on pentacene in *p*-terphenyl 212 (1993) 71
- Cromack, K.R., D.W. Werst, M.V. Barnabas and A.D. Trifunac, Low-temperature study of radical cations of quadricyclane and norbornadiene in Na-ZSM-5 zeolites 218 (1994) 485
- Crosby, G.A., see J.A. Burt 220 (1994) 493
- Crowell, R.A. and E.L. Chronister, A photon echo study of pentacene in naphthalene at high pressure 216 (1993) 293



- Crystall, B., see I.D.W. Samuel 213 (1993) 472
- Culver, J.P., M. Li, L.G. Jahn, R.M. Hochstrasser and A.G. Yodh, Vibrational response of surface adsorbates to femtosecond substrate heating 214 (1993) 431
- Curtiss, L.A., K. Raghavachari and J.A. Pople, The accurate determination of enthalpies of formation 214 (1993) 183
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- Czuchaj, E., F. Rebentrost, H. Stoll and H. Preuss, Calculation of the interaction energies for the ZnHg and ZnCd system 212 (1993) 534
- Czuchaj, E., F. Rebentrost, H. Stoll and H. Preuss, Adiabatic potential curves for the KZn and KCd excimers 218 (1994) 454



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- D'Angelo, M., G. Onori and A. Santucci, Study of aggregation of *n*-butoxyethanol in water by compressibility and surface tension measurements 220 (1994) 59
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- Darmanyan, A.P., Mechanism of singlet oxygen interaction with solvent removing prohibition of the radiative  ${}^1\Delta_g \rightarrow {}^3\Sigma_g^-$  transition in oxygen 215 (1993) 477
- Das, A.K., see T.K. Ghosh 218 (1994) 433
- Das, G.P., A.T. Yeates and D. Dudis, Vibronic contribution to static molecular hyperpolarizabilities 212 (1993) 671
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- Davis, H.F., P.I. Ionov, S.I. Ionov and C. Wittig, Picosecond resolution measurements of NO<sub>3</sub> unimolecular decomposition. The NO + O<sub>2</sub> channel 215 (1993) 214
- De Andrés, J., see A. Aguilar 220 (1994) 267
- Debnath, R. and J. Chaudhuri, Coordination structure and the bonding properties of UV-laser-induced photo-generated Cu(II) in a monovalent copper containing silica glass 217 (1994) 357
- De Boer, J.L., S. van Smaalen, V. Petricek, M. Dusek, M.A. Verheijen and G. Meijer, Hexagonal close-packed C<sub>60</sub> 219 (1994) 469
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- Degli Esposti, C., F. Tamassia, G. Cazzoli and P. De Natale, High-resolution Fourier transform spectroscopy of the  $\nu_1$  fundamental band of nitrosyl bromide 214 (1993) 531
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- Denton, A.R., C.G. Gray and D.E. Sullivan, Orientational ordering of surfactant monolayers adsorbed at the air-water interface. Structural model and fit to neutron reflectivity data 219 (1994) 310
- Depaemelaere, S., L. Viaene, M. Van der Auweraer, F.C. De Schryver, R.M. Hermant and J.W. Verhoeven, Non-radiative decay processes of the intramolecular charge transfer state in a rigid bichromophoric system 215 (1993) 649
- Depero, L.E. and F. Parmigiani, A study of the electronic structure of decagonal  $\text{Al}_{70}\text{Ni}_{15}\text{Co}_{15}$  quasi-crystal 214 (1993) 208
- De Proft, F. and P. Geerlings, The effect of electron correlation on the shell structure of atoms 220 (1994) 405
- DeRose, P., H.L. Dai and P.Y. Cheng, Degenerate four-wave mixing spectroscopy of the (glyoxal)<sub>2</sub> van der Waals complex 220 (1994) 207
- De Santis, A., A. Gregori and D. Rocca, The range of the local order in a model of diatomic liquid 213 (1993) 239
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- Dibble, T.S. and J.S. Francisco, An ab initio study of the reaction of atomic fluorine and chlorine with trifluoroacetaldehyde 215 (1993) 409
- Dibble, T.S. and J.S. Francisco,  $\text{FNO}_2$ : improving calculated structures at the second-order Møller-Plesset level of theory 215 (1993) 423
- Di Bella, S., G. Lanza and I.L. Fraga, Equilibrium geometries and harmonic vibrational frequencies of lanthanum trihalides  $\text{LaX}_3$  ( $\text{X} = \text{F}, \text{Cl}$ ). A relativistic effective core potential ab initio MO study 214 (1993) 598
- DiCarlo, J., see C.-H. Park 213 (1993) 196
- Dietz, K., C. Schmidt, M. Warken and B.A. Heß, Explicit construction of a convergent MBPT series for the  $^1\Delta$  state of  $\text{C}_2$  and the  $\text{H}_2$  ground state at large bond distance 220 (1994) 397
- Diewald, M. and H.R. Brand, Chemically driven convection. A simple model 216 (1993) 566
- Dikanov, S.A., C. Burgard and J. Hüttermann, Determination of the hyperfine coupling with the remote nitrogen in the  $\text{VO}^{2+}$ -(imidazole)<sub>4</sub> complex by ESEEM spectroscopy 212 (1993) 493
- Ding, G., W. Yang, W. Sun, D. Xu, G. He and N. Lou, The product polarization of chemiluminescent reactions of orbital aligned  $\text{Ca}(^1\text{P}_1)$  with  $\text{CH}_3\text{I}$  and  $\text{C}_2\text{H}_5\text{I}$  220 (1994) 1
- Ding, L.N., M.A. Young, P.D. Kleiber and W.C. Stwalley, Photofragmentation spectroscopy of  $\text{Mg}_2\text{CO}_2^+$  212 (1993) 499
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- Dippel, O., V. Brandl, H. Bässler, R. Danieli, R. Zamboni and C. Taliani, Energy-dependent branching between fluorescence and singlet exciton dissociation in sexithienyl thin films 216 (1993) 418

- Dirksen, G.J., see G. Blasse 215 (1993) 363
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- Dolson, D.A. and D.S. West, Infrared fluorescence observations of electronic to vibrational energy transfer from  $\text{Cl}^*[3\text{p}^5(^2\text{P}_{1/2})]$  to  $\text{SO}_2$  216 (1993) 258
- Domcke, W., see A.L. Sobolewski 211 (1993) 82
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- Donley, E.A. and D.P. Shelton, Hyperpolarizabilities measured for interacting molecular pairs 215 (1993) 156
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- Douhal, A., F. Amat-Guerri, A.U. Acuña and K. Yoshihara, Picosecond vibrational relaxation in the excited-state proton-transfer of 2-(3'-hydroxy-2'-naphthyl)benzimidazole 217 (1994) 619
- Douhal, A. and R. Sastre, Room-temperature triple proton transfer of 7-hydroxyquinoline and stabilization of its ground-state keto tautomer in a polymeric matrix 219 (1994) 91
- Douhal, A., see F. Lahmani 220 (1994) 235
- Douin, S., J.-H. Fillion, M. Bonneau, P. Bréchignac, D. Furio, D. Gauyacq, M. Horani and N. Shafizadeh, Dual time-of-flight photoelectron-photoion spectrometry on a magnetic bottle-molecular beam apparatus 216 (1993) 215
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- Drickamer, H.G., see J.M. Lang 214 (1993) 310
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- Duncan, J.L., see M.M. Law 212 (1993) 172  
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- Eades, R.A., see C. Sosa 211 (1993) 265
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- Egsgaard, H., see E.L. Thomsen 215 (1993) 257
- Ehbrecht, M., M. Faerber, F. Rohmund, V.V. Smirnov, O. Stelmakh and F. Huisken,  $CO_2$ -laser-driven production of carbon clusters and fullerenes from the gas phase 214 (1993) 34
- Eilers, H., U. Hömmerich, S.M. Jacobsen and W.M. Yen, The near-infrared emission of  $Cr:Mn_2SiO_4$  and  $Cr:MgCaSiO_4$  212 (1993) 109
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- Ellert, Ch., see Th. Reiners 215 (1993) 357
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- Engert, C., S. Umapathy, W. Kiefer and H. Hamaguchi, Dynamic structure of charge carrier in polyaniline by near-infrared excited resonance Raman spectroscopy 218 (1994) 87
- Enomoto, M., see J.S. Ahn 215 (1993) 336
- Eriksson, L.A., J. Wang and R.J. Boyd, The effect of a neon matrix on the hyperfine structure of  $CH_4^+$ . A model study 211 (1993) 88
- Eriksson, L.A., see J. Kong 217 (1994) 24

- Erman, P., A. Karawajczyk, E. Rachlew-Källne, C. Strömholm, J. Larsson, A. Persson and R. Zerne, Direct determination of the ionization potential of CO by resonantly enhanced multiphoton ionization mass spectroscopy 215 (1993) 173
- Ermler, W.C., see D. Andrae 220 (1994) 341
- Ernst, H., D. Freude and I. Wolf, Multinuclear solid-state NMR studies of Brønsted sites in zeolites 212 (1993) 588
- Ernst, M.C., A.F. Sax and J. Kalcher, Intramolecular H-transfer reactions in  $\text{Si}_2\text{H}_n$  (for  $n=3-5$ ) 216 (1993) 189
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- Ernst, R.R., see M. Tomaselli 214 (1993) 1
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- Fahlman, M., D. Beljonne, M. Lögdlund, R.H. Friend, A.B. Holmes, J.L. Brédas and W.R. Salaneck, Experimental and theoretical studies of the electronic structure of Na-doped poly(para-phenylenevinylene) 214 (1993) 327
- Fain, B., T.C. Chang, H.T. Liou, D.Y. Yang, K.L. Huang, M.-C. Chan and S.H. Lin, Dual-frequency pump-probe time-resolved spectroscopy 216 (1993) 551
- Fairbrother, D.H., see S.J. Garrett 219 (1994) 409
- Falcetta, M.F. and P.E. Siska, Ab initio study of the long-range interaction between  $\text{He}^+$  and  $\text{H}_2$  213 (1993) 531
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- Fárník, M., Z. Dolejšek, Z. Herman and V.E. Bondybey, Beam scattering investigation of hydride-ion transfer processes. Reaction of  $\text{CH}_3^+$  and  $\text{CD}_3^+$  with  $\text{C}_2\text{H}_6$  216 (1993) 458
- Farrelly, D. and M.D. Emmel, Semiclassical quantization of doubly excited intrashell resonances of the helium atom 217 (1994) 520
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- Fedrigo, S., W. Harbich, J. Belyaev and J. Buttet, Evidence for electronic shell structure of small silver clusters in the optical absorption spectra 211 (1993) 166
- Fehér, M., A. Rohrbacher, J.P. Maier and A. Miklós, Optoacoustic spectroscopy of short-lived molecules 211 (1993) 171
- Fehér, M., see T. Pasinszki 215 (1993) 395
- Fehér, M. and P.A. Martin, Ab initio calculations of the properties of  $\text{NO}^+$  in its ground electronic state  $X^1\Sigma$  215 (1993) 565
- Feldchtein, F., see S. Hess 216 (1993) 247
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- Felder, P., X. Yang and J.R. Huber, Photodissociation of nitric acid in a cold molecular beam at 193 nm 215 (1993) 221
- Felder, P., see G.P. Morley 219 (1994) 195
- Feldhaus, J., see M. Neeb 212 (1993) 205
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- Feng, P.Y., see K. Balasubramanian 214 (1993) 85
- Feng, S., D. Feng and C. Deng, Theoretical studies on the structures and reactivity of silylenoids. III. The structures and isomerization of silylenoid  $\text{H}_2\text{SiNaF}$  214 (1993) 97
- Fenistein, S., see S. Jullien 212 (1993) 340
- Fernández, A. and A. Belinky, Learning to fold a random RNA chain 212 (1993) 201
- Fernández-Serra, P., see V. Botella 219 (1994) 497
- Ferrari, A.M., E. Garrone and P. Ugliengo, Ab initio study of the gas-phase equilibrium between  $(\text{H}_2\text{O})_4$  and  $(\text{H}_2\text{O})_8$  212 (1993) 644



- Ferrarini, A., G.R. Luckhurst, P.L. Nordio and S.J. Roskilly, Understanding the unusual transitional behaviour of liquid crystal dimers 214 (1993) 409
- Ferrario, M., M.L. Klein and I.R. McDonald, Dynamical behavior of the azide ion in protic solvents 213 (1993) 537
- Ferrero, J.C., see R.A. Bollati 218 (1994) 159
- Ferretti, A. and A. Lami, Optical properties of pyrazine-bridged ruthenium chains by the two-band Hubbard Hamiltonian 220 (1994) 327
- Feyereisen, M.W., see O. Vahtras 213 (1993) 514
- Fichou, D., see J.-M. Nunzi 215 (1993) 114
- Fiedler, A., J. Hrušák, W. Koch and H. Schwarz, The energetical and structural properties of  $\text{FeO}^+$ . An application of multireference perturbation theory 211 (1993) 242
- Field, R.W., see R. Liyanage 216 (1993) 544
- Field, R.W., see G.M. Schmid 219 (1994) 331
- Field, T.A. and J.H.D. Eland, Lifetimes of metastable molecular doubly charged ions 211 (1993) 436
- Figari, G., see V. Magnasco 213 (1993) 17
- Figuera, J.M., see M. Castillejo 214 (1993) 227
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- Fink, E.H., see O. Shestakov 211 (1993) 473
- Fink, E.H., see R. Breidohr 218 (1994) 13
- Finney, L.M., A. Borrmann and C.C. Martens, Nonstationary time series analysis of intramolecular energy transfer 214 (1993) 159
- Finnila, A.B., M.A. Gomez, C. Sebenik, C. Stenson and J.D. Doll, Quantum annealing: a new method for minimizing multidimensional functions 219 (1994) 343
- Fiorini, C., see J.-M. Nunzi 219 (1994) 349
- Fiory, A.T., see R.C. Haddon 218 (1994) 100
- Fischer, P.R., J.L. Daschbach and G.L. Richmond, Surface second harmonic studies of  $\text{Si}(111)/\text{electrolyte}$  and  $\text{Si}(111)/\text{SiO}_2/\text{electrolyte}$  interfaces 218 (1994) 200
- Fitzgerald, G., see C. Sosa 211 (1993) 265
- Fleissner, G., A. Hallbrucker and E. Mayer, Raman spectroscopic evidence for increasing contact-ion pairing in the glassy states of "dilute" aqueous calcium nitrate solutions 218 (1994) 93
- Fletcher, J., see P. Bond 211 (1993) 649
- Fletcher, T.R., see K. Ravichandran 217 (1994) 375
- Flügge, J., see P. Botschwina 215 (1993) 681
- Fockenberg, Ch., H. Saathoff and R. Zellner, A laser photolysis/LIF study of the rate constant for the reaction  $\text{CF}_3\text{O} + \text{O}_3 \rightarrow \text{products}$  218 (1994) 21
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- Forest, S.E. and R.L. Kuczkowski, The microwave spectrum of cyclopropane·ammonia. A novel structure for cyclopropane complexes 218 (1994) 349
- Forrest, S.R., see E.I. Haskal 219 (1994) 325
- Fort, A., see M. Lequan 213 (1993) 71
- Fortunelli, A. and A. Painelli, Interacting electrons in the solid state: the role of orbital relaxation 214 (1993) 402
- Foss, M., F. Besenbacher, C. Klink and I. Stensgaard, Deuterium-induced restructuring of  $\text{Cu}(100)$  215 (1993) 535

- Fournier, T., see T.-H. Tran-Thi 213 (1993) 139
- Fowler, G.J.S., see H. van der Laan 212 (1993) 569
- Fowler, P.W., H.M. Kelly and A.J. Sadlej, Electric and magnetic properties of the phosphorus trifluoride molecule 212 (1993) 659
- Fowler, P.W., H.M. Kelly and R.J.C. Brown, The nitrogen Sternheimer antishielding factor in the ammonium ion 216 (1993) 200
- Fox, D.J., see B.G. Johnson 218 (1994) 595
- Fraenkel, R. and Y. Haas, Photolysis of ICN in a cryogenic matrix 214 (1993) 234
- Fraenkel, R. and Y. Haas, A molecular dynamics simulation of NBr trapping in an argon matrix 220 (1994) 77
- Fragalà, I.L., see S. Di Bella 214 (1993) 598
- Fraissard, J., see A. Gedeon 219 (1994) 440
- Francisco, J.S., Z. Li, A. Bradley and A.E.W. Knight, Degradation of alternative halocarbons. Decomposition pathways of trifluoroethoxy radicals 214 (1993) 77
- Francisco, J.S., Z. Li, M.R. Hand and I.H. Williams, Theoretical characterisation of the lowest  $n \rightarrow \pi^*$  electronic state of  $\text{CF}_2\text{O}$ . Is it planar or non-planar? 214 (1993) 591
- Francisco, J.S. and Y. Su, An ab initio study of the reaction between FO radicals and  $\text{H}_2\text{O}$  215 (1993) 58
- Francisco, J.S., see T.S. Dibble 215 (1993) 409, 423
- Francisco, J.S. and Y. Su, A computational study of the reaction between FO radicals and methane 215 (1993) 417
- Francisco, J.S., Ab initio investigation of the decomposition of trifluoromethanol into carbonyl fluoride and hydrogen fluoride 218 (1994) 401
- Francisco, J.S., see J.A. Montgomery Jr. 220 (1994) 391
- Franken, K.A. and C.E. Dykstra, Quantum Monte Carlo vibrational analysis of the nitrogen–water complex 220 (1994) 161
- Frankevich, E., Y. Maruyama and H. Ogata, Mobility of charge carriers in vapor-phase grown  $\text{C}_{60}$  single crystal 214 (1993) 39
- Frankevich, E.L., see M.M. Triebel 214 (1993) 315, 321
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- Freiberg, A., A. Ellervee, P. Kukk, A. Laisaar, M. Tars and K. Timpmann, Pressure effects on spectra of photosynthetic light-harvesting pigment–protein complexes 214 (1993) 10
- Freiser, B.S., see S. Afzaal 218 (1994) 254
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- Friedrich, K.A. and G.L. Richmond, Surface second harmonic generation studies of stepped Ag(111) electrode surfaces 213 (1993) 491
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- Fuentealba, P. and A. Savin, A test for the Wilson-Levy correlation energy functional 217 (1994) 566
- Fuglesang, C.D., see D.A. Baugh 219 (1994) 207
- Fujii, M., see S. Tanabe 215 (1993) 347
- Fujimoto, N., see Y. Saito 212 (1993) 379
- Fujitani, Y., T. Miyazaki, N.M. Masaki, Y. Aratono and E. Tachikawa, Effect of rotational quantum states ( $J=0, 1$ ) on the tunneling reaction  $H_2 + T \rightarrow H + HT$  in xenon-hydrogen mixtures at 77 K 214 (1993) 301
- Fujito, T., see T. Fujiwara 212 (1993) 81
- Fujiwara, T., A. Ramamoorthy, K. Nagayama, K. Hioka and T. Fujito, Dipolar HOHAHA under MAS conditions for solid-state NMR 212 (1993) 81
- Fujiwara, Y., see H. Mukaihata 211 (1993) 140
- Fujiwara, Y., M. Mukai, T. Tamura, Y. Tanimoto and M. Okazaki, A laser flash photolysis study of the effect of intense magnetic fields on the photoreaction of benzophenone in SDS micellar solution 213 (1993) 89
- Fujiwara, Y., see R. Takasu 217 (1994) 478
- Fukazawa, N., see S. Yamamoto 215 (1993) 323
- Fukazawa, N., see S. Hashimoto 219 (1994) 445
- Fukazawa, N., H. Fukumura, H. Masuhara and J. Prochorow, A picosecond diffuse reflectance laser photolysis study on phenanthrene-pyromellitic dianhydride charge-transfer crystal 220 (1994) 461
- Fuke, K., see H. Umemoto 214 (1993) 271
- Fukumura, H., see S. Yamamoto 215 (1993) 323
- Fukumura, H., see S. Hashimoto 219 (1994) 445
- Fukumura, H., see N. Fukazawa 220 (1994) 461
- Fulara, J., M. Jakobi and J.P. Maier, Electronic and infrared spectra of  $C_{60}^+$  and  $C_{60}^-$  in neon and argon matrices 211 (1993) 227
- Fulde, P., see J. Gräfenstein 215 (1993) 611
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- Gadonas, R., see R. Gagel 217 (1994) 228
- Gadre, S.R. and R.N. Shirsat, Comment on "Computing molecular electrostatic potentials with the PRISM algorithm" 218 (1994) 593
- Gagel, R., R. Gadonas and A. Laubereau, Evidence for biexcitons and dynamic Stark effect in J-aggregates from femtosecond spectroscopy 217 (1994) 228
- Gale, J.D., C.R.A. Catlow and J.R. Carruthers, An ab initio study of methanol adsorption in zeolites 216 (1993) 155
- Gallazzi, A.M., see M. Nisoli 220 (1994) 64
- Gal'pern, E.G., I.V. Stankevich, A.L. Chistykov and L.A. Chernozatonskii, Carbon nanotubes with metal inside: electron structure of tubelenes  $[\text{Li}@\text{C}_{24}]_n$  and  $[\text{K}@\text{C}_{36}]_n$  214 (1993) 345
- Galvão, D.S., see R.H. Baughman 211 (1993) 110
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- Ganteför, G. and W. Eberhardt, Shell structure and s-p hybridization in small aluminum clusters 217 (1994) 600
- García, F., see G.G. Lazarev 212 (1993) 319
- García de la Vega, J.M. and B. Miguel, Single-exponent Slater function expansions of the He atom is orbital and its isoelectronic series (Chem. Phys. Letters 207 (1993) 270). Erratum 212 (1993) 420
- García Solé, J., see U. Caldiño G. 213 (1993) 84
- García-Sucre, M., see J.L. Paz 217 (1994) 333
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- Garrett, S.J., D.H. Fairbrother, V.P. Holbert, E. Weitz and P.C. Stair, Multiphoton ionization mechanisms in  $\text{CH}_3\text{I}$  and  $\text{CD}_3\text{I}$  219 (1994) 409
- Garrett, W.R., see R.B. Jones 212 (1993) 451
- Garrone, E., see A.M. Ferrari 212 (1993) 644
- Gartstein, Yu.N. and E.M. Conwell, High-field hopping mobility of polarons in disordered molecular solids. A Monte Carlo study 217 (1994) 41
- Gasparoli, A., see G. Karwasz 211 (1993) 529
- Gatti, C., see V. Bonačić-Koutecký 213 (1993) 522
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- Ge, M. and K. Sattler, Observation of fullerene cones 220 (1994) 192
- Gedanken, A., see E. Sominska 213 (1993) 117
- Gedeon, A. and J. Fraissard,  $^{129}\text{Xe}$  NMR of AgX, CuX, ZnX and CdX zeolites. Comparative study of  $nd^{10}$  element-xenon interactions 219 (1994) 440
- Geen, H., J.J. Titman and H.W. Spiess, Heteronuclear magnetization transfer in rapidly spinning solids 213 (1993) 145
- Geerlings, P., see F. de Proft 220 (1994) 405
- Gehlen, M.H., Fluorescence quenching in clusters of reverse micelles 212 (1993) 362
- Geil, B. and G. Hinze, Influence of data treatment on the shape of  $^2\text{H}$  NMR  $T_1$  curves 216 (1993) 51
- Gejo, T., M. Takayanagi, T. Kono and I. Hanazaki, Photodissociation dynamics of acetaldehyde. Vibrational energy distribution in the photofragment HCO 218 (1994) 343
- Gelb, L.D. and R.M. Lynden-Bell, Force oscillations and liquid structure in simulations of an atomic force microscope tip in a liquid 211 (1993) 328
- George, S.M., see D.R. Haynes 214 (1993) 50

- George, T.F., see I. Last 216 (1993) 599
- Gerber, Ch., see J.K. Gimzewski 213 (1993) 401; 217 (1994) 589
- Gertner, I., see I. Ben-Itzhak 212 (1993) 467
- Ghose, K.B., P.G. Nair and S. Pal, Implementation of a stationary coupled-cluster response method 211 (1993) 15
- Ghosh, A. and J. Almlöf, The ultraviolet photoelectron spectrum of free-base porphyrin revisited. The performance of local density functional theory 213 (1993) 519
- Ghosh, T.K., A.K. Das and P.K. Mukherjee, New resonances in a dynamic polarizability calculation 218 (1994) 433
- Gibbons, V.C., see J. Baker 215 (1993) 163
- Gierer, M., see H. Bludau 219 (1994) 452
- Giesbergen, C.P.M., C. Terletski, G. Frei, H.U. Güdel and M. Glasbeek, Optically detected magnetic resonance spectroscopy of rhodium(III) mixed-chelate complexes 213 (1993) 597
- Gilbert, J.V., A.M. Zarubaiko and S. Lantz, UV absorption spectrum of low-temperature matrix-isolated NFCl radicals 220 (1994) 19
- Gildemeister, J.M. and G.K. Wertheim, Electronic properties of  $Cs_xC_{60}$  films for the complete range of stoichiometries 220 (1994) 181
- Gilibert, M., see A. Aguilar 220 (1994) 267
- Gill, D., see Z. Chernia 212 (1993) 57
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- Gill, P.M.W., B.G. Johnson and J.A. Pople, A simple yet powerful upper bound for Coulomb integrals 217 (1994) 65
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- Gillan, M.J., see I. Štich 212 (1993) 617
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- Gimzewski, J.K., S. Modesti, Ch. Gerber and R.R. Schlittler, Observation of a new Au(111) reconstruction at the interface of an adsorbed  $C_{60}$  overlayer 213 (1993) 401
- Gimzewski, J.K., Ch. Gerber, E. Meyer and R.R. Schlittler, Observation of a chemical reaction using a micromechanical sensor 217 (1994) 589
- Giro, G., J. Kalinowski, P.D. Marco, V. Fattori and G. Marconi, Absorption tail photoconductivity in solid films of  $C_{60}$  211 (1993) 580
- Glasbeek, M., see C.P.M. Giesbergen 213 (1993) 597
- Głaz, W., J. Yang, J.D. Poll and C.G. Gray, Complex plane method for interaction-induced spectra in 3D systems 218 (1994) 183
- Glish, G.L., see L.D. Hulett Jr. 216 (1993) 236
- Goddard, J.D., see C.G. Joslin 213 (1993) 377
- Goldanskii, V.I. and F. Parak, Some still open questions of relaxational CO-heme rebinding 219 (1994) 379
- Goldberg, N., D. Sülzle and H. Schwarz, The gas-phase generation and characterization of butatrienylidene  $H_2CCCC$ : by neutralization-reionization mass spectrometry 213 (1993) 593
- Goldman, S., see C.G. Joslin 211 (1993) 587; 213 (1993) 377; 215 (1993) 144
- Gomez, M.A., see A.B. Finnila 219 (1994) 343
- Gong, M., Y. Bao, R.S. Urdahl and W.M. Jackson, LIF measurements of radiative lifetimes of the  $C_2(B' \ ^1\Sigma_g^+)$  state 217 (1994) 210
- Gong, M.-X., see R. Huang 216 (1993) 108, 115
- González, M., see A. Aguilar 220 (1994) 267
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- Göpel, W., see P. Lemoine 220 (1994) 177
- Gorbunov, B.Z., E.L. Zapadinsky, K.K. Sabelfeld and M. Ataev, Influence of inhomogeneity and fluctuations of supersaturation on heterogeneous nucleation 215 (1993) 31
- Gordon, E.B., V.V. Khmelenko and O.S. Rzhevsky, Critical phenomena in electron drift through condensed rare gases 217 (1994) 605
- Gordon, M.S., see T.L. Windus 216 (1993) 375
- Gordon, R.D., J. Michael Hollas, P.J.A. Ribeiro-Claro and J.J.C. Teixeira-Dias,  $\text{CF}_3$ -torsional potentials of 2-aminobenzotrifluoride in the  $S_0$  and  $S_1$  electronic states from fluorescence spectra in a supersonic jet 211 (1993) 392
- Gordon, R.J., see R. Liyanage 216 (1993) 544
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- Gorse, C., see G. Colonna 213 (1993) 5
- Gosine, J.N., see X. Song 217 (1994) 216
- Goto, M. and S. Saito, Submillimeter-wave spectra of the PH and PD radicals in the  $^3\Sigma^-$  state 211 (1993) 443
- Gotschy, B., see A. Skiebe 220 (1994) 138
- Gotts, N.G., see G. von Helden 212 (1993) 241
- Goubert, L., G.D. Billing, E. Desoppere and W. Wieme, Semiclassical calculation of the probabilities for collision-induced vibrational transitions in  $\text{Ar}_2^*$  219 (1994) 360
- Govoni, D.E., J.A. Booze, A. Sinha and F.F. Crim, The non-resonant signal in laser-induced grating spectroscopy of gases 216 (1993) 525
- Goyal, P.S., S.V.G. Menon, B.A. Dasannacharya and V. Rajagopalan, Role of van der Waals forces on small angle neutron scattering from ionic micellar solutions 211 (1993) 559
- Grabmaier, B.C., see E. Bayer 216 (1993) 228
- Graener, H., see K. Wolfrum 213 (1993) 41
- Gräfenstein, J., H. Stoll and P. Fulde, Computation of the valence band of diamond by means of local increments 215 (1993) 611
- Graja, A., see N.D. Kushch 215 (1993) 137
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- Gray, C.G., see C.G. Joslin 211 (1993) 587; 213 (1993) 377; 215 (1993) 144
- Gray, C.G., see W. Głaz 218 (1994) 183
- Gray, C.G., see A.R. Denton 219 (1994) 310
- Gray, J.A. and R. Trebino, Two-photon-resonant four-wave-mixing spectroscopy of atomic hydrogen in flames 216 (1993) 519
- Grayson, M. and W.T. Raynes, Electric field effects on the magnetic shielding of first and second row nuclei in some simple molecules 214 (1993) 473
- Grayson, M. and W.T. Raynes, Electric field effects on proton magnetic shielding in some binary hydrides 218 (1994) 270
- Grebner, D., see D.V. Lap 211 (1993) 135
- Green, P.G., see P. Dupré 212 (1993) 555
- Greenlief, C.M., see L.A. Keeling 217 (1994) 136
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- Grimley, T.B., The quantum theory of the rates of sticking and desorption 214 (1993) 447
- Grimme, S., S.D. Peyerimhoff, S. Bartram, F. Vögtle, A. Breest and J. Hormes, Experimental and theoretical study of the circular dichroism spectra of oxa- and thia-[2.2]metacyclopentane 213 (1993) 32



- Grinberg, O.Ya., see S.D. Chemerisov 218 (1994) 353
- Grishanin, B.A., see V.D. Vachev 215 (1993) 306
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- Groombridge, C.J., see P.J. Barrie 219 (1994) 491
- Gross, H., Y. He, M. Quack, A. Schmid and G. Seyfang, Time-resolved detection of reaction products in the infrared laser chemistry of sulfoxides:  $C_2H_4SO$ ,  $(CH_3)_2SO$ ,  $(CD_3)_2SO$  213 (1993) 122
- Grunze, M., see Ch. Zubrägel 219 (1994) 127
- Gryziński, M., Dynamical model of the molecular bond 217 (1994) 481
- Gu, X., L.A. Muñoz, Y. Ishikawa and B.R. Weiner, Isotope effects and wavelength dependence in the rotational state distributions of the diatomic photofragments SH and SD from the photodissociation of  $H_2S$  and  $D_2S$  211 (1993) 65
- Güdel, H.U., see C.P.M. Giesbergen 213 (1993) 597
- Guillaud, G. and J. Simon, Transient properties of nickel phthalocyanine thin film transistors 219 (1994) 123
- Guillot, J.-P., see R. Azria 220 (1994) 417
- Guo, H., see M.H.M. Janssen 214 (1993) 281
- Guo, H., L. Liu and K. Lao, Non-perturbative time-dependent quantal dynamics of superexchange in electron transfer processes 218 (1994) 212
- Guo, J., see X. Mao 218 (1994) 249
- Gurav, A.S., T.T. Kodas, L.-M. Wang, E.I. Kauppinen and J. Joutsensaari, Generation of nanometer-size fullerene particles via vapor condensation 218 (1994) 304
- Gurioli, M., see M. Nikl 220 (1994) 14
- Gustavsson, T., see P. Hébert 213 (1993) 345
- Gütlich, P., see Th. Buchen 220 (1994) 262
- Gutman, I., D. Todorović and M. Vučković, A variant of the Frank chiral amplification model 216 (1993) 447
- Gutman, I., J. Brunvoll, B.N. Cyvin, E. Brendsdal and S.J. Cyvin, Essentially disconnected fully-acenoids, and fully-arenoid hydrocarbons 219 (1994) 355
- Güttler, F., see M. Croci 212 (1993) 71
- Güttler, F., T. Irngartinger, T. Plakhotnik, A. Renn and U.P. Wild, Fluorescence microscopy of single molecules 217 (1994) 393
- Gvishi, R., R. Reisfeld and Z. Burshtein, Excited-state absorption in red perylimide dye in solution 212 (1993) 463
- Gvishi, R., R. Reisfeld and Z. Burshtein, Spectroscopy and laser action of the "red perylimide dye" in various solvents 213 (1993) 338

- Haaland, P.D., see J. Holtgrave 215 (1993) 548
- Haarer, D., see R.B. Altmann 216 (1993) 281
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- Haddon, R.C., A.S. Perel, R.C. Morris, S.-H. Chang, A.T. Fiory, A.F. Hebard, T.T.M. Palstra and G.P. Kochanski, Electrical resistivity and stoichiometry of  $K_xC_{60}$ ,  $Rb_xC_{60}$ , and  $Cs_xC_{60}$  films 218 (1994) 100
- Haffer, C.M. and M. Kunst, Computational simulations of charge carrier kinetics in a-Si:H 211 (1993) 203
- Hagler, T.W., Nonparallel transition dipole moments and the polarization dependence of electroabsorption in nonoriented conjugated polymer films 218 (1994) 195
- Hähner, G., see Ch. Zubrägel 219 (1994) 127
- Hall, J., O. Saksager and I. Chorkendorff, Dissociative chemisorption of  $O_2$  on Cu(100). Effects of mechanical energy transfer and recoil 216 (1993) 413
- Hall, R.J., N.A. Burton, I.H. Hillier and P.E. Young, Tautomeric equilibria in 2-hydroxypyridine and in cytosine. An assessment of density functional methods, including gradient corrections 220 (1994) 129
- Hallbrucker, A., see G. Fleissner 218 (1994) 93
- Halonen, L., see M. Saarinen 219 (1994) 181
- Halvick, P., see L. Bonnet 216 (1993) 11
- Halvorson, C., R. Wu, D. Moses, F. Wudl and A.J. Heeger, Third harmonic generation spectra of degenerate ground state derivatives of poly(1,6-heptadiyne) 212 (1993) 85
- Halvorson, C. and A.J. Heeger, Two-photon absorption spectrum of oriented trans-polyacetylene 216 (1993) 488
- Hamaguchi, H., see T. Tahara 217 (1994) 369
- Hamaguchi, H., see C. Engert 218 (1994) 87
- Hamai, S., N. Tamai and H. Masuhara, Effects of the solid/liquid interface on the excimer formation of pyrene in toluene containing poly(methyl methacrylate). A time-resolved total internal reflection fluorescence study 213 (1993) 407
- Hamanoue, K., see T. Nakayama 213 (1993) 581; 215 (1993) 622; 220 (1994) 219
- Hamilton, P.A., see J. Baker 213 (1993) 297; 215 (1993) 163
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- Hammonds, K.D., I.R. McDonald and J.-P. Ryckaert, Conformer distribution and the kinetics of trans-gauche isomerization in a model of liquid *n*-octane 213 (1993) 27
- Han, K.-L., see R.-J. Li 220 (1994) 281
- Hanazaki, I., see Y. Mori 211 (1993) 421
- Hanazaki, I., Fragment rotational excitation due to the parent rotation in the dissociation of molecules 218 (1994) 151
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- Haneman, D. and H. Tributsch, d-state contribution to STM. Structure of van der Waals surfaces ( $TaSe_2$ ,  $Mo_{0.5}W_{0.5}Se_2$ ) and relevance for catalysis 216 (1993) 81

- Hansen, K., C. Yeretdzian and R.L. Whetten, A simple rate equation for fullerene coalescence 218 (1994) 462
- Hara, H., see S.A. Dzuba 214 (1993) 621
- Harbich, W., see S. Fedrigo 211 (1993) 166
- Harbola, M.K., Electric dipole polarizabilities for helium-like ions from correlated wavefunctions. A density-functional approach 217 (1994) 461
- Harcourt, R.D., Valence bond studies of the barrier to rotation around the N-N bond of N<sub>2</sub>O<sub>4</sub> 218 (1994) 175
- Harder, H., H.-W. Nicolaisen, H. Dreizler and H. Mäder, One- and two-dimensional Fourier transform spectroscopy in the microwave and radiofrequency range of trifluoromethane in the vibrational state  $\nu_6 = 1$  214 (1993) 265
- Hartke, B. and E.A. Carter, Ab initio molecular dynamics simulated annealing at the generalized valence bond level. Application to a small nickel cluster 216 (1993) 324
- Hase, H. and Y. Miyatake, Electronic spectra of C<sub>70</sub> anions produced in  $\gamma$ -irradiated organic glasses at 77 K 215 (1993) 141
- Haselbach, E., see E. Vauthey 215 (1993) 264
- Hashimoto, S., N. Fukazawa, H. Fukumura and H. Masuhara, Observation and characterization of excimer emission from anthracene included in NaX zeolite 219 (1994) 445
- Hashizume, T., see Y. Kohno 214 (1993) 603
- Hashizume, T., see X.-D. Wang 216 (1993) 409
- Haskal, E.I., Y. Zhang, P.E. Burrows and S.R. Forrest, Finite size effects observed in the fluorescence of ultrathin crystalline organic films grown by organic molecular beam deposition 219 (1994) 325
- Hasselbrink, E., see K.W. Kolasinski 219 (1994) 113
- Hatherly, P.A., see D.M. Smith 216 (1993) 493
- Hatta, N. and K. Murata, Very long graphitic nano-tubules synthesized by plasma-decomposition of benzene 217 (1994) 398
- Hättig, C., see J.G. Ángyán 219 (1994) 267
- Haugen, H.K., see L.H. Andersen 217 (1994) 204
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- Hayashi, H., see Y. Nakamura 217 (1994) 387
- Hayashi, K., see M. Yagi 211 (1993) 179
- Hayashi, M., R. Islampour and S.H. Lin, The calculation of single-vibronic level rate constants for displaced-distorted potential surfaces 213 (1993) 465
- Hayden, B.E., see A.E. Wiskerke 216 (1993) 93
- Hayden, B.E., see D.A. Butler 217 (1994) 423
- Haynes, D.R., A. Tokmakoff and S.M. George, Temperature-dependent absolute fluorescence quantum yield of C<sub>60</sub> multilayers 214 (1993) 50
- He, G., see G. Ding 220 (1994) 1
- He, G.-Z., see R.-J. Li 220 (1994) 281
- He, Y., see H. Gross 213 (1993) 122
- He, Y., M. Quack, R. Ranz and G. Seyfang, Diode laser detection of iodine atom hyperfine transitions during and after infrared multiphoton excitation and dissociation of CF<sub>3</sub>I with short pulse CO<sub>2</sub> lasers 215 (1993) 228
- Head, J.D. and S. Jin, Efficient tools for theoretically investigating surface structure applied to Al on graphite 212 (1993) 32
- Head-Gordon, M., see R.J. Rico 213 (1993) 224; 218 (1994) 139



- Head-Gordon, M., R.J. Rico, M. Oumi and T.J. Lee, A doubles correction to electronic excited states from configuration interaction in the space of single substitutions 219 (1994) 21
- Head-Gordon, M. and T. Head-Gordon, Analytic MP2 frequencies without fifth-order storage. Theory and application to bifurcated hydrogen bonds in the water hexamer 220 (1994) 122
- Head-Gordon, T., see M. Head-Gordon 220 (1994) 122
- Hebard, A.F., see R.C. Haddon 218 (1994) 100
- Heber, O., see I. Ben-Itzhak 212 (1993) 467
- Hébert, P., G. Baldacchino, T. Gustavsson and J.-C. Mialocq, Sub-picosecond fluorescence study of the LDS 751 dye molecule in ethanol 213 (1993) 345
- Hediger, S., B.H. Meier and R.R. Ernst, Cross polarization under fast magic angle sample spinning using amplitude-modulated spin-lock sequences 213 (1993) 627
- Heeger, A.J., see C. Halvorson 212 (1993) 85; 216 (1993) 488
- Heeger, A.J., see B. Kraabel 213 (1993) 389
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- Heinemann, C. and W. Thiel, Ab initio study on the stability of diaminocarbenes 217 (1994) 11
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- Helenius, V., see E. Laitinen 218 (1994) 73
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- Henderson, C.C., C.M. Rohlfing and P.A. Cahill, Theoretical studies of selected  $C_{60}H_2$  and  $C_{70}H_2$  isomers 213 (1993) 383
- Henderson, D., see W. Schmickler 216 (1993) 424
- Heninger, M., see S. Jullien 212 (1993) 340
- Henriksen, N.E. and B. Amstrup, Coherent control of HOD photodissociation dynamics in the first absorption band 213 (1993) 65
- Hepburn, J.W., see A. Mank 219 (1994) 169
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- Hernandez, R. and W.H. Miller, Semiclassical transition state theory. A new perspective 214 (1993) 129
- Herrero, C.P., Framework dependence of atom ordering in tectosilicates. A lattice gas model 215 (1993) 587
- Herrero, V.J., see F.J. Aoiz 211 (1993) 72; 218 (1994) 422
- Herreros, B. and J. Klinowski, Synthesis of zeolites from sodium silicoglycolate, a 5-coordinate silicon compound 220 (1994) 478
- Hershberger, J.F., see J. Park 218 (1994) 537
- Hertel, N., see L.H. Andersen 217 (1994) 204
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- Heß, B.A., see K. Dietz 220 (1994) 397
- Hess, S., F. Feldchtein, A. Babin, I. Nurgaleev, T. Pullerits, A. Sergeev and V. Sundström, Femtosecond energy transfer within the LH2 peripheral antenna of the photosynthetic purple bacteria *Rhodobacter sphaeroides* and *Rhodospseudomonas palustris* LL 216 (1993) 247

- Heully, J.-L., see D. Maynau 211 (1993) 625
- Heully, J.L., see J. Meller 218 (1994) 276
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- Higgins, D.A., R.R. Naujok and R.M. Corn, Second harmonic generation measurements of molecular orientation and coadsorption at the interface between two immiscible electrolyte solutions 213 (1993) 485
- Higo, J., see T. Yamato 219 (1994) 155
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- Hillier, I.H., see R.J. Hall 220 (1994) 129
- Hilpert, G., H. Linnartz, M. Havenith, J.J. ter Meulen and W.L. Meerts, Tunable infrared and far-infrared direct absorption spectroscopy of molecular ions in a supersonic jet expansion 219 (1994) 384
- Hinchliffe, A. and H.J. Soscun Machado, Ab initio study of the static dipole polarizability of naphthalene 214 (1993) 64
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- Hirsch, G., see H.-P. Liebermann 214 (1993) 381
- Hiyama, M. and S. Iwata, Theoretical assignment of the vibronic bands in the photoelectron spectra of  $N_2$  below 30 eV 211 (1993) 319
- Ho, K.M., see X.Q. Wang 214 (1993) 193; 217 (1994) 199
- Hồ, M., R.P. Sagar, J.M. Pérez-Jordá, V.H. Smith Jr. and R.O. Esquivel, A numerical study of molecular information entropies 219 (1994) 15
- Hobza, P., see J. Vacek 220 (1994) 85
- Hochstrasser, R.M., see J.P. Culver 214 (1993) 431
- Hoeft, J. and T. Törring, The microwave rotational spectrum of  $X^2\Sigma^+ YO$  215 (1993) 367
- Hoeft, J. and K.P.R. Nair, Millimeter wave rotational spectrum of gallium monofluoride 215 (1993) 371
- Hof, M., see H. Lanig 220 (1994) 423
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- Hoffman, D.K., see W. Zhu 217 (1994) 73
- Hoffman, D.K., see D.J. Kouri 220 (1994) 312
- Hoffmann, E. and A. Schweiger, Stimulated echo description of coherent Raman beat EPR spectroscopy 220 (1994) 467
- Hoffmann, H., see K.L. Walther 212 (1993) 96
- Hofmann, H.-J., see R. Cimiraglia 217 (1994) 430
- Hogreve, H., The ground state geometry of the  $Ne_3^+$  trimer 215 (1993) 72
- Hohm, U., Modelling of the long-range part of the invariants of the incremental pair polarizability tensor  $\Delta\hat{\alpha}$  211 (1993) 498

- Hohmann, J., G. Müller, G. Schönnenbeck and F. Stuhl, Temperature-dependent quenching of  $O_2(b^1\Sigma_g^+)$  by  $H_2$ ,  $D_2$ ,  $CO_2$ ,  $HN_3$ ,  $DN_3$ ,  $HNCO$  and  $DNCO$  217 (1994) 577
- Holbert, V.P., see S.J. Garrett 219 (1994) 409
- Holden, J.M., see Y. Wang 211 (1993) 341; 217 (1994) 413
- Holden, J.M., P. Zhou, X.-X. Bi, P.C. Eklund, S. Bandow, R.A. Jishi, K. Das Chowdhury, G. Dresselhaus and M.S. Dresselhaus, Raman scattering from nanoscale carbons generated in a cobalt-catalyzed carbon plasma 220 (1994) 186
- Holme, T.A. and T.N. Truong, A test of density functional theory for dative bonding systems 215 (1993) 53
- Holmes, A.B., see I.D.W. Samuel 213 (1993) 472
- Holmes, A.B., see M. Fahlman 214 (1993) 327
- Holmes, J.L., F.P. Lossing and P.M. Mayer, The effects of methyl substitution on the structure and thermochemistry of the cyanomethyl radical and cation 212 (1993) 134
- Holovko, M.F., see Yu.V. Kalyuzhnyi 215 (1993) 1
- Holtgrave, J., K. Riehl, D. Abner and P.D. Haaland, Ion chemistry in tetraethylorthosilicate  $(C_2H_5O)_4Si$  215 (1993) 548
- Holtom, G.R., see R. Knochenmuss 215 (1993) 188
- Hömmerich, U., see H. Eilers 212 (1993) 109
- Hömmerich, U., H. Eilers, W.M. Yen and H.R. Verdún, The optical center  $M_nO_4^{3-}$  in  $Y_2SiO_5:Mn$ , X (X=Al, Ca) 213 (1993) 163
- Honigmann, M., see Y. Li 212 (1993) 185
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- Hormes, J., see S. Grimme 213 (1993) 32
- Horoyski, P.J. and M.L.W. Thewalt,  $C_{70}$  vibrational frequencies obtained from singlet oxygen photoluminescence 217 (1994) 409
- Horsewill, A.J., see S. Clough 211 (1993) 637
- Hoshino, K., T. Naganuma, K. Watanabe, A. Nakajima and K. Kaya, Ionization potentials of gold-sodium  $(Au_nNa_m)$  bimetallic clusters 211 (1993) 571
- Hoshino, K., see A. Nakajima 214 (1993) 22
- Hotokka, M., see O.-P. Sairanen 215 (1993) 353
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- Howard, S.T. and K. Woźniak, The effect of electron correlation on the structure and properties of the benzenium ion 212 (1993) 1
- Howdle, S.M. and V.N. Bagratashvili, The effects of fluid density on the rotational Raman spectrum of hydrogen dissolved in supercritical carbon dioxide 214 (1993) 215
- Hrbek, J., see J.A. Rodriguez 220 (1994) 486
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- Huang, K.L., see B. Fain 216 (1993) 551
- Huang, R., J. Wu, M.-X. Gong, A. Saury and E. Carrasquillo M., Direct observation of vibrational relaxation in highly excited HCN 216 (1993) 108
- Huang, R., J. Wu, M.-X. Gong, A. Saury and E. Carrasquillo M., Vibrational state-to-state resolution in the collisional relaxation of a highly vibrationally excited polyatomic: HCN 216 (1993) 115



- Huang, Y. and S.-I. Chu, Study of the photoabsorption spectrum of diamagnetic Rydberg atoms without the need of using full eigenvectors 211 (1993) 601
- Huang, Y., W. Zhu, D.J. Kouri and D.K. Hoffman, A general time-to-energy transform of wavepackets. Time-independent wavepacket-Schrödinger and wavepacket-Lippmann-Schwinger equation (Chem. Phys. Letters 206 (1993) 96). Erratum 213 (1993) 209
- Huang, Y., W. Zhu, D.J. Kouri and D.K. Hoffman, Analytic continuation of the polynomial representation of the full, interacting time-independent Green function 214 (1993) 451
- Huang, Y., see W. Zhu 217 (1994) 73
- Huang, Y., see D.J. Kouri 220 (1994) 312
- Huber, J.R., see M.-A. Thelen 213 (1993) 275
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- Hubrich, M., G.G. Maresch and H.W. Spiess, Pulsed electron nuclear double resonance study of molecular motions of radicals in a high-strength liquid-crystalline polymer 218 (1994) 81
- Huché, M., see M. Lequan 213 (1993) 71
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- Hulett Jr., L.D., D.L. Donohue, J. Xu, T.A. Lewis, S.A. McLuckey and G.L. Glish, Mass spectrometry studies of the ionization of organic molecules by low-energy positons 216 (1993) 236
- Hunter, C.N., see H. van der Laan 212 (1993) 569
- Hurley, M.D., see T.J. Wallington 211 (1993) 41; 213 (1993) 442; 218 (1994) 34
- Hurwitz, Y., Y. Rudich and R. Naaman, Reactant rotational energy effect on energy distribution in products. The role of the electronic angular momentum 215 (1993) 674
- Hüttermann, J., see S.A. Dikanov 212 (1993) 493
- Huuang, J.-S., see W.-D. Cheng 216 (1993) 353
- Huzinaga, S. and M. Klobukowski, Well-tempered Gaussian basis sets for the calculation of matrix Hartree-Fock wavefunctions 212 (1993) 260
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- Ibuki, K., see T. Nakayama 215 (1993) 622; 220 (1994) 219
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- I'Haya, Y.J. and S. Kanosue, Solvent dependence of excited molecule-free radical interactions studied by means of time-resolved electron spin resonance 216 (1993) 231
- I'Haya, Y.J., see K. Kobayashi 219 (1994) 53
- Iijima, T., Anharmonicity of the OH...O hydrogen bond in liquid water 217 (1994) 503
- Ikeda, H., see H. Umemoto 214 (1993) 271
- Ikeda, R., see N. Kimura 220 (1994) 40
- Ikemoto, I., see K. Kikuchi 216 (1993) 67
- Ikeura, H., K. Tanaka, T. Sekiguchi and K. Obi, Observation of neutral products of a soft X-ray stimulated etching reaction in the SF<sub>6</sub>/a-SiO<sub>2</sub> absorption system 217 (1994) 131
- Ikeyama, T. and T. Azumi, Triplet spin-sublevel selectivity of the S<sub>1</sub>-T<sub>1</sub> intersystem crossing in trans-stilbene 212 (1993) 551
- Illas, F., see C. Sousa 215 (1993) 97
- Illas, F., see J. Rubio 217 (1994) 283
- Imamura, A., see Y. Kohno 214 (1993) 603
- Inaba, R., K. Tominaga, M. Tasumi, K.A. Nelson and K. Yoshihara, Observation of homogeneous vibrational dephasing in benzonitrile by ultrafast Raman echoes 211 (1993) 183
- Infante, G., see G. Polzonetti 214 (1993) 333
- Iogansen, A.A., O.M. Sarkisov, E.V. Zimont, J.A. Seetula, R.S. Timonen and S. Cheskis, Formation of vibrationally excited OH radicals in the O(<sup>1</sup>D) + H<sub>2</sub>S reaction 212 (1993) 604
- Ionov, P.I., see H.F. Davis 215 (1993) 214
- Ionov, S.I., see H.F. Davis 215 (1993) 214
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- Ishida, T., A classical cross-section calculation for Penning ionization with multi-exit channels. N<sub>2</sub>-He\*(2 <sup>3</sup>S) → N<sub>2</sub><sup>+</sup>(<sup>2</sup>Σ<sub>g</sub><sup>+</sup>, <sup>2</sup>Π<sub>u</sub>, <sup>2</sup>Σ<sub>u</sub><sup>+</sup>) + He + e<sup>-</sup> 211 (1993) 1
- Ishii, J., T. Matsui, K. Tsukiyama and K. Uehara, Observation of the A <sup>2</sup>Σ<sup>+</sup> ← X <sup>2</sup>Π<sub>3/2</sub> transition of nitric oxide with two-photon degenerate four-wave mixing 220 (1994) 29
- Ishikawa, M. and Y. Maruyama, Femtosecond spectral hole-burning of crystal violet in methanol. New evidence for ground state conformers 219 (1994) 416
- Ishikawa, Y., see X. Gu 211 (1993) 65
- Ishikawa, Y., Comment on "Segmented contractions of relativistic Gaussian basis sets" 212 (1993) 547
- Ishikawa, Y., Ab initio study of the structure and ionization potential of aluminum-sodium bimetallic cluster, Al<sub>2</sub>Na 213 (1993) 527
- Ishikawa, Y., see V. Keshari 218 (1994) 406
- Islampour, R., see M. Hayashi 213 (1993) 465
- Ito, A., T. Morikawa and T. Takahashi, Photo-induced polymerization and oxidation of C<sub>60</sub> observed by photoelectron spectroscopy 211 (1993) 333
- Ito, M., see M. Mimuro 213 (1993) 576
- Ito, S., see H. Sekiya 215 (1993) 499
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- Itoh, M., see H. Mukaihata 211 (1993) 140
- Itoh, M., see R. Takasu 217 (1994) 478
- Ivanov, A.I. and V.A. Mikhaylova, The effect of a magnetic field on outer-sphere electron transfer 212 (1993) 697
- Iwata, S., see M. Hiyama 211 (1993) 319

- Jackson, W.M., see M. Gong 217 (1994) 210
- Jackson, W.M., see X. Song 217 (1994) 216
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- Jacobs, A., H.-R. Volpp and J. Wolfrum, Reaction dynamics, OH energy partitioning, and OH product angular momentum alignment studies:  $\text{H} + \text{H}_2\text{O} \rightarrow \text{OH} + \text{H}_2$  versus  $\text{H} + \text{CO}_2 \rightarrow \text{OH} + \text{CO}$  218 (1994) 51
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- James, A.M., P. Kowalczyk and B. Simard, First observation of the VNb molecule 216 (1993) 512
- James, G.K., see I. Kanik 211 (1993) 523
- Janicke, M., see R.G. Larsen 214 (1993) 220
- Jansen, G., B.A. Hess and P.E.S. Wormer, Theoretical investigation of the rovibrational fine-structure spectrum of Ar-NH in its electronic ground state 214 (1993) 103
- Jansen, G., see J.G. Ángyán 219 (1994) 267
- Janssen, M.H.M., M. Dantus, H. Guo and A.H. Zewail, Femtosecond reaction dynamics of Rydberg states. Methyl iodide 214 (1993) 281
- Janszky, J., P. Adam, An.V. Vinogradov and T. Kobayashi, Vibrational state shaping for selective laser chemistry 213 (1993) 368
- Jaque, F., see U. Caldiño G. 213 (1993) 84
- Jasinski, J.M., Formation of gas-phase silyl radicals in the atomic hydrogen etching of silicon 211 (1993) 564
- Jasra, R.V., N.V. Choudary, K.V. Rao, G.C. Pandey and S.G.T. Bhat, Far-IR spectroscopic studies on zeolite NaCaA 211 (1993) 214
- Jaszunski, M., T. Helgaker, K. Ruud, K.L. Bak and P. Jørgensen, MCSCF calculations of nitrogen NMR shielding constants using London atomic orbitals 220 (1994) 154
- Jayannavar, A.M., see G.V. Raviprasad 220 (1994) 353
- Jayatilaka, D., Analytic SCF third and fourth derivatives with model potentials 212 (1993) 18
- Jeevarajan, A.S., L.D. Kispert and X. Wu, Spectroelectrochemistry of carotenoids in solution 219 (1994) 427
- Jemmis, E.D., see G. Subramanian 217 (1994) 296
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- Jensen, V.R. and P.E.M. Siegbahn, The Ziegler-Natta olefin insertion reaction for cationic metals 212 (1993) 353
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- Johnson, A.E., S. Kumazaki and K. Yoshihara, Pump-probe spectroscopy and exciton dynamics of J aggregates at high pump intensities 211 (1993) 511
- Johnson, B.G., see K. Raghavachari 214 (1993) 357; 220 (1994) 385
- Johnson, B.G. and M.J. Frisch, Analytic second derivatives of the gradient-corrected density functional energy. Effect of quadrature weight derivatives 216 (1993) 133
- Johnson, B.G., see P.M.W. Gill 217 (1994) 65
- Johnson, B.G., J.A. Pople, P.M.W. Gill and D.J. Fox, Reply to Comment on "Computing molecular electrostatic potentials with the PRISM algorithm" 218 (1994) 595
- Johnson, B.G., P.M.W. Gill and J.A. Pople, A rotationally invariant procedure for density functional calculations 220 (1994) 377
- Johnson, K.H., see T.S. Smit 212 (1993) 525
- Johnson, M.A., see M.A. Buntine 216 (1993) 471
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- Jones, A.C., M.J. Dale, G.A. Keenan and P.R.R. Langridge-Smith, Photoionisation and photodissociation of laser-vaporised metallotetraphenylporphyrins 219 (1994) 174
- Jones, J.D., see D.A. Butler 217 (1994) 423
- Jones, R.B., S.L. Allman, K. Tang, W.R. Garrett and C.H. Chen, Neutralization of negatively charged oligonucleotides 212 (1993) 451
- Jongma, R.T., see G. Meijer 217 (1994) 112
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- Joslin, C.G., J. Yang, C.G. Gray, S. Goldman and J.D. Poll, Infrared rotation and vibration-rotation bands of endohedral fullerene complexes.  $K^+@C_{60}$  211 (1993) 587
- Joslin, C.G., C.G. Gray, J.D. Goddard, S. Goldman, J. Yang and J.D. Poll, Infrared rotation and vibration-rotation bands of endohedral fullerene complexes.  $He@C_{60}$  213 (1993) 377
- Joslin, C.G., C.G. Gray, S. Goldman, J. Yang and J.D. Poll, Raman spectra of endohedral fullerenes.  $Li^+@C_{60}$  215 (1993) 144
- Joutsensaari, J., see A.S. Gurav 218 (1994) 304
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- Jovanic, B.R., Lj.D. Zekovic and B. Radenkovic, Theoretical calculations of the pressure-induced shift of a photoacoustic phase signal in alexandrite ( $BeAl_2O_4:Cr^{3+}$ ) 216 (1993) 47
- Judeinstein, P., P.W. Oliveira, H. Krug and H. Schmidt, Dynamics of the sol-gel transition in organic-inorganic nanocomposites 220 (1994) 35
- Jug, K., see T. Kar 214 (1993) 615
- Jullien, S., J. Lemaire, S. Fenistein, M. Heninger, G. Mauclaire and R. Marx, Radiative lifetimes of  $Xe^+$  and  $Kr^+$  in their  $^2P_{1/2}$  spin-orbit states 212 (1993) 340
- Jungwirth, P. and R. Zahradník, Is the water-induced potential of mean torsion of *n*-butane transferable to longer *n*-alkanes? 212 (1993) 211
- Jungwirth, P. and R. Zahradník, The entropy driven hydrophobic effect as a function of solute-solvent interactions. A molecular dynamics study 217 (1994) 319

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- Kajzar, F., C. Taliani, R. Danieli, S. Rossini and R. Zamboni, Wave-dispersed third-order nonlinear optical properties of  $C_{60}$  thin films 217 (1994) 418
- Kalcher, J. and A.F. Sax, Stabilities and stationary points for singlet and triplet states of the  $Si_2H^-$  anion 215 (1993) 601
- Kalcher, J., see M.C. Ernst 216 (1993) 189
- Kalinowski, J., see G. Giro 211 (1993) 580
- Kalontarov, L.I., Kinetic regularities for laser-induced thermal reactions of polymers 217 (1994) 222
- Kalyuzhnyi, Yu.V., I.A. Protsykevych and M.F. Holovko, Solution of the associative Percus-Yevick approximation for the  $n$ -component mixture of dimerizing hard spheres 215 (1993) 1
- Kalyuzhnyi, Yu.V. and V. Vlady, Integral equation theory for highly asymmetric electrolyte solutions 215 (1993) 518
- Kamalov, V.F., I.A. Struganova and K. Yoshihara, Time-resolved emission spectra of the BIC J-aggregate at low temperature 213 (1993) 559
- Kamalov, V.F., I.A. Struganova, T. Tani and K. Yoshihara, Temperature dependence of superradiant emission of BIC J-aggregates 220 (1994) 257
- Kamarás, K., L. Akselrod, S. Roth, A. Mittelbach, W. Hönlé and H.G. von Schnering, The orientational phase transition in  $C_{60}$  films followed by infrared spectroscopy 214 (1993) 338
- Kaminskii, A.A., see U. Caldino G. 213 (1993) 84
- Kandori, H., K. Yoshihara, H. Tomioka, H. Sasabe and Y. Shichida, Comparative study of primary photochemical events of two retinal proteins, bacteriorhodopsin and halorhodopsin, by use of subpicosecond time-resolved spectroscopy 211 (1993) 385
- Kandori, H. and H. Sasabe, Excited-state dynamics of a protonated Schiff base of all-trans retinal in methanol probed by femtosecond fluorescence measurement 216 (1993) 126
- Kanematsu, Y., see J.S. Ahn 215 (1993) 336
- Kanik, I., J.M. Ajello and G.K. James, Extreme ultraviolet emission spectrum of  $CO_2$  induced by electron impact at 200 eV 211 (1993) 523
- Kanosue, S., see Y.J. I'Haya 216 (1993) 231
- Kaplan, I.G., see R. Santamaria 218 (1994) 395
- Kar, T. and K. Jug, The remarkable stability of the  $LiBH_2$  and  $HBeBH_2$  dimers. B=B double bond or multi-center bonds? 214 (1993) 615
- Kar, T., P.K. Nandi and A.B. Sannigrahi, Bonding in beryllium carbonyls 220 (1994) 133
- Karawajczyk, A., see P. Erman 215 (1993) 173
- Karna, S.P., A "direct" time-dependent coupled perturbed Hartree-Fock-Roothaan approach to calculate molecular (hyper)polarizabilities 214 (1993) 186
- Karthäuser, J., see I.R. Sims 211 (1993) 461
- Karwasz, G., R.S. Brusa, A. Gasparoli and A. Zecca, Total cross-section measurements for  $e^-$ -CO scattering: 80-4000 eV 211 (1993) 529
- Kasemo, B., see M. Rinnemo 211 (1993) 60
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- Kawai, A., Y. Kobori and K. Obi, Time-resolved ESR spectra of the  $\alpha$ -hydroxybenzyl-amine complex 215 (1993) 203
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- Kedzierski, W., J.B. Atkinson and L. Krause, Laser-induced fluorescence from the  $^3\Pi_u(4^3P, 4^3P)$  state of  $Zn_2$  215 (1993) 185
- Kedzierski, W., J. Supronowicz, A. Czajkowski, M.J. Hinek, J.B. Atkinson and L. Krause, The rotationally resolved  $G0_u^+ \leftarrow A0_g^+$  electronic spectrum of the  $(^{202}Hg)_2$  excimer 218 (1994) 314
- Keeling, L.A., L. Chen, C.M. Greenlief, A. Mahajan and D. Bonser, Direct evidence for  $\beta$ -hydride elimination on Si(100) 217 (1994) 136
- Keenan, G.A., see A.C. Jones 219 (1994) 174
- Keita, B., L. Nadjo, R. Céolin, V. Agafonov, D. André, H. Szwarc, J. Dugué, C. Fabre, A. Rassat and P.-Y. Sizaret, Scanning tunneling microscopy study of the surface of  $C_{60}$  decagonal crystals grown from  $n$ -hexane 215 (1993) 125
- Kelly, C., H.W. Sidebottom, J. Treacy and O.J. Nielsen, Reactions of  $CF_3O$  radicals with selected alkenes and aromatics under atmospheric conditions 218 (1994) 29
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- Keshari, V. and Y. Ishikawa, Ab initio Monte Carlo simulated annealing method 218 (1994) 406
- Keshavamurthy, S. and W.H. Miller, Semi-classical correction for quantum-mechanical scattering 218 (1994) 189
- Khan, A., Theoretical studies of the clathrate structures of  $(H_2O)_{20}$ ,  $H^+(H_2O)_{20}$  and  $H^+(H_2O)_{21}$  217 (1994) 443
- Khanna, S.N. and P. Jena, Reactivity of hydrogen with open and closed shell clusters 218 (1994) 383
- Khanna, S.N. and P. Jena, Designing ionic solids from metallic clusters 219 (1994) 479
- Kharlamov, A.A., L.A. Chernozatonskii and A.A. Dityat'ev, Two states of  $C_{60}$  film at the air/water interface 219 (1994) 457
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- Kikuchi, K., S. Suzuki, Y. Nakao, N. Nakahara, T. Wakabayashi, H. Shiromaru, K. Saito, I. Ikemoto and Y. Achiba, Isolation and characterization of the metallofullerene  $LaC_{82}$  216 (1993) 67
- Kilcoyne, A.L.D., see M. Neeb 212 (1993) 205
- Kim, B. and K. Yoshihara,  $^3\Delta-^1\Sigma^+$  transition of  $RbCs$  observed in a very cold molecular beam 212 (1993) 271
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- Kim, J., B.J. Mhin, S.J. Lee and K.S. Kim, Entropy-driven structures of the water octamer 219 (1994) 243
- Kim, K. and K.D. Jordan, Theoretical calculation of the height of the barrier for OH rotation in phenol 218 (1994) 261

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- Kimura, N., H. Ohki, R. Ikeda and M. Yamashita, Valence structure of one-dimensional halogen bridged  $-\text{Pt}-\text{Pt}-\text{X}-\text{Pt}-\text{Pt}-\text{X}-$  type complexes studied by  $^{31}\text{P}$  solid NMR 220 (1994) 40
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- Klein, U.K.A., J. Mastromarino, Z.H. Yamani and A. Suwaiyan, Fluorescence demodulation spectroscopy. A new method of determining fluorescence decays using two beating ring dye lasers 217 (1994) 80
- Klein, U.K.A., J. Mastromarino and A. Suwaiyan, Rotational level lifetimes and self-quenching of  $^{127}\text{I}_2$  by fluorescence demodulation spectroscopy 217 (1994) 86
- Kleindienst, H., see A. Lüchow 216 (1993) 359
- Kleindienst, H., A. Lüchow and H.-P. Merckens, Accurate upper and lower bounds for some excited S states of the He atom 218 (1994) 441
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- Kneipp, H., K. Kneipp and F. Seifert, Surface-enhanced hyper-Raman scattering (SEHRS) and surface-enhanced Raman scattering (SERS) by means of mode-locked Ti:sapphire laser excitation 212 (1993) 374

- Kneipp, K., see H. Kneipp 212 (1993) 374
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- Knochenmuss, R., G.R. Holtom and D. Ray, Proton transfer reaction rates as a probe of size-dependent properties of large water clusters 215 (1993) 188
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- Knuth, E.L. and H.-G. Rubahn, Cross sections for rotational relaxation in alkali dimer molecular beams 213 (1993) 1
- Knuts, S., see Y. Luo 213 (1993) 356
- Kobayashi, K., see S. Nagase 214 (1993) 57
- Kobayashi, K., T. Sano and Y.J. I'Haya, Quasi-particle energy band structure and core-electron transition energy calculation for two-dimensional hexagonal boron nitride 219 (1994) 53
- Kobayashi, R., H. Koch, P. Jørgensen and T.J. Lee, Comparison of coupled-cluster and Brueckner coupled-cluster calculations of molecular properties 211 (1993) 94
- Kobayashi, R., O. Bludský, H. Koch and P. Jørgensen, Quartic coupled cluster force fields for the diazene isomers 215 (1993) 576
- Kobayashi, R., H. Koch and P. Jørgensen, Calculation of frequency-dependent polarizabilities using coupled-cluster response theory 219 (1994) 30
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- Kobe, K., H. Kühling, S. Rutz, E. Schreiber, J.P. Wolf, L. Wöste, M. Broyer and Ph. Dugourd, Time-resolved observation of molecular pseudorotation in Na<sub>3</sub> 213 (1993) 554
- Kobori, Y., see A. Kawai 215 (1993) 203
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- Koch, H. and E. Dalgaard, Linear superposition of optimized non-orthogonal Slater determinants for singlet states 212 (1993) 193
- Koch, R., B. Burg, K. Schmidt, K.H. Rieder, E. Schwarz and K. Christmann, Oxygen adsorption on Co(10 $\bar{1}$ 0). The structure of p(2 $\times$ 1)2O 220 (1994) 172
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- Kohno, Y., K. Maekawa, T. Tsuchioka, T. Hashizume and A. Imamura, A molecular orbital study on the effects of electron correlation on the unique N-N bond in nitramines 214 (1993) 603
- Koizumi, H., Photoionization quantum yield for liquid squalane and squalene estimated from photoelectron emission yield 219 (1994) 137
- Kolasinski, K.W., F. Cemic and E. Hasselbrink, O<sub>2</sub>/Pd(111). Clarification of the correspondence between thermal desorption features and chemisorption states 219 (1994) 113
- Kolb, D., see T. Baştuğ 211 (1993) 119
- Kolbuszewski, M. and J.S. Wright, Thermodynamically stable diatomic dications: MgN<sup>2+</sup>, MgO<sup>2+</sup>, MgF<sup>2+</sup> and MgNe 218 (1994) 338
- Kolesnick, R.E., see G.D. Billing 215 (1993) 571
- Kolibiar, M., M. Foltin and T.D. Märk, Molecular dynamics simulation of Xe<sup>+</sup> ion collisions with Ar<sub>29</sub> and Ne<sub>29</sub> clusters 219 (1994) 252



- Komaromi, I. and J.M.J. Tronchet, The geometry of the  $\text{H}_2\text{NO}$  radical: do the quantum mechanical results converge? 215 (1993) 444
- Kominami, K., see K. Sakoda 215 (1993) 488; 216 (1993) 270
- Kompa, K.L., see K.L. Bintz 215 (1993) 455
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- Kondepudi, D.K. and C. Sabanayagam, Secondary nucleation that leads to chiral symmetry breaking in stirred crystallization 217 (1994) 364
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- Kong, J., L.A. Eriksson and R.J. Boyd, A density functional theory study of the hyperfine structures of the atoms B to O and the species  $\text{NH}_2$  and  $\text{NH}_3^+$  217 (1994) 24
- Konishi, Y., see A. Nakajima 214 (1993) 22
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- Kono, H., Extraction of eigenstates from an optically prepared state by a time-dependent quantum-mechanical method. Toward simulation of "intermediate case" radiationless transitions 214 (1993) 137
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- Konrat, R., G. Zieger and H. Sterk, Directed coherence transfer in nuclear magnetic resonance. Two-dimensional in-phase multiplets in selective correlation spectroscopy 212 (1993) 78
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- Koperski, J., J.B. Atkinson and L. Krause, The  $0_u^+(6\ ^3\text{P}_1) \leftarrow \text{X}0_g^+$  spectrum of  $\text{Hg}_2$  excited in a supersonic jet 219 (1994) 161
- Koppe, S., T. Laurent, P.D. Naik, H.-R. Volpp, J. Wolfrum, T. Arusi-Parpar, I. Bar and S. Rosenwaks, Absolute rate constants and reactive cross sections for the reactions of  $\text{O}(^1\text{D})$  with molecular hydrogen and deuterium 214 (1993) 546
- Kornyshev, A.A. and K.M. Robinson, Interfacial electronic profile from X-ray reflectivity 219 (1994) 132
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- Koubi, L., M. Blain, E. Cohen de Lara and J.-M. Leclercq, Vibrational frequency shifts of diatomic molecules in interaction with a  $\text{Na}^+$  cation by ab initio calculations. Comparison with experiment on  $\text{H}_2$  and  $\text{N}_2$  adsorbed in NaA zeolite 217 (1994) 544
- Kouri, D.J., see Y. Huang 213 (1993) 209; 214 (1993) 451
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- Kouyaté, D., see S. Bachir 213 (1993) 54
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- Kozankiewicz, B., Migration of CT triplet excitons in TCNB-biphenyl and TCNB-HMB crystals 217 (1994) 91
- Kraabel, B., C.H. Lee, D. McBranch, D. Moses, N.S. Sariciftci and A.J. Heeger, Ultrafast photoinduced electron transfer in conducting polymer-buckminsterfullerene composites 213 (1993) 389
- Kraemer, W.P. and W. Koch, A CASSCF-CI study of the ground and low-lying excited electronic states of  $\text{C}_2\text{H}_2^+$  212 (1993) 631

- Kraka, E. and D. Cremer, Ortho-, meta-, and para-benzyne. A comparative CCSD(T) investigation 216 (1993) 333
- Kraka, E. and D. Cremer, Ortho-, meta-, and para-benzyne. A comparative CCSD (T) investigation (Chem. Phys. Letters 216 (1993) 333). Addendum 219 (1994) 160
- Krämer, U., see K.L. Walther 212 (1993) 96
- Krause, H. and H.J. Neusser, The van der Waals modes of the (benzene-Ar)<sup>+</sup> complex studied by mass selective pulsed field threshold ionization 213 (1993) 603
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- Krishnamurthy, M. and D. Mathur, Collision-induced dissociation of oriented CO<sup>+</sup> ions. Probing potential energy curves by ion collision spectrometry 216 (1993) 203
- Krishnan, P.N., J.O. Jensen and L.A. Burke, Theoretical study of water clusters. II. Hexamer 217 (1994) 311
- Kronseider, C., see C. Berg 216 (1993) 465
- Kroto, H.W. and D.R.M. Walton, Stable derivatives of small fullerenes 214 (1993) 353
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- Krüger, S. and N. Rösch, Embedding effects on core level shifts of surface cluster models 216 (1993) 435
- Krzysztofowicz, A.M. and C. Szmytkowski, Electron scattering from methyl bromide. Absolute total cross section measurements 219 (1994) 86
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- Kühling, H., see K. Kobe 213 (1993) 554
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- Kukolich, S.G. and S.M. Sickafoose, The microwave spectrum and Mn-H bond length for HMn(CO)<sub>5</sub> 215 (1993) 168
- Kumar, G.R., C.P. Safvan, F.A. Rajgara and D. Mathur, Intense laser field ionisation of CS<sub>2</sub> at 532 nm. Does dissociation precede ionisation? 217 (1994) 626
- Kumazaki, S., see A.E. Johnson 211 (1993) 511
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- Kuppermann, A. and Y.-S.M. Wu, The geometric phase effect shows up in chemical reactions (Chem. Phys. Letters 205 (1993) 577). Erratum 213 (1993) 636
- Kurita, S., see J. Takeda 220 (1994) 443
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- Kushch, N.D., I. Majchrzak, W. Ciesielski and A. Graja, Preparation and spectral properties of C<sub>60</sub>S<sub>16</sub>·0.5C<sub>6</sub>H<sub>5</sub>Cl and C<sub>60</sub>·0.5C<sub>6</sub>H<sub>5</sub>Cl compounds 215 (1993) 137
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- Laaksonen, L. and J.B. Rosenholm, Molecular dynamics simulations of the water/octanoate interface in the presence of micelles 216 (1993) 429
- LaBrake, D. and E. Weitz, H atom mobilities in xenon matrices. Dependence on matrix morphology 211 (1993) 430
- Lacks, D.J. and S. Kais, Statistical model for delocalized  $\pi$  bonding in the  $C_{60}$  molecule 218 (1994) 229
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- Laitinen, E., P. Ruuskanen-Järvinen, U. Rempel, V. Helenius and J.E.I. Korppi-Tommola, Rotation correlation time as a measure of microviscosity of excited state isomerization reactions of three cyanine dyes in *n*-alcohol solutions 218 (1994) 73
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- Lang, J.M., A.A. Dadali and H.G. Drickamer, Luminescence of the flexible dye molecule julolidinemalononitrile in polymer matrices at pressures above 40 kbar 214 (1993) 310
- Langenberg, J.D., see J.C. Pinegar 212 (1993) 458
- Langhoff, S.R. and C.W. Bauschlicher Jr., A theoretical study of the electric dipole moment function of SiO 211 (1993) 305
- Langhoff, S.R., see C.W. Bauschlicher Jr. 211 (1993) 312; 216 (1993) 341
- Langridge-Smith, P.R.R., see A.C. Jones 219 (1994) 174
- Lanig, H., M. Hof, T. Stahl and F.W. Schneider, Intramolecular deactivation of substituted quinolinium cations. Time-resolved fluorescence and semi-empirical calculations 220 (1994) 423
- Lantz, K.O. and V. Vaida, Direct absorption spectroscopy of the first excited electronic band of jet-cooled  $H_2S$  215 (1993) 329
- Lantz, S., see J.V. Gilbert 220 (1994) 19
- Lanza, G., see S. Di Bella 214 (1993) 598
- Lanzisera, D.V. and J.J. Valentini, Surprising positive correlation between rotational and vibrational excitation in the  $H + CDCl_3 \rightarrow HD + CCl_3$  reaction 216 (1993) 122
- Lao, K., see H. Guo 218 (1994) 212
- Lap, D.V., D. Grebner, S. Rentsch and H. Naarmann, Femtosecond-spectroscopic investigations on bithiophene, terthiophene and tetrathiophene in solution 211 (1993) 135
- Lara, F., see G.G. Lazarev 212 (1993) 319
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- Larin, A.V., S.V. Poljanskii and D.N. Trubnikov, Assignment of the torsional structure of the  $0_0^0$  band of the electronic transition  $A_{1g} \rightarrow B_{2u}$  in van der Waals clusters of type  $C_6H_6-X$  ( $X = N_2, CO_2, CO$ ) 213 (1993) 619
- Larsen, R.G., J. Shore, K. Schmidt-Rohr, L. Emsley, H. Long, A. Pines, M. Janicke and B.F. Chmelka, NMR study of xenon dynamics and energetics in Na-A zeolite 214 (1993) 220
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- Last, I. and T.F. George, Multiple ionization of rare gas clusters. Theoretical treatment 216 (1993) 599
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- Lazarev, G.G., V.L. Kuskov, F. Lara, F. García, A. Rieker and P. Tordo, The role of dopant geometry in the photoinduced formation of radical pairs in crystals of 2,6-di-tert-butyl-4-methylphenol and 2,6-di-tert-butylphenol 212 (1993) 319
- Lazarev, G.G., V.L. Kuskov, K. Laukenmann and A. Angerhofer, Spin dynamics of neutral radical pairs in single crystals of di-tert-butyl-pyrocatechol doped with tetrakis(*t*-butyl)-phenoxazin 215 (1993) 375
- Lazzeretti, P., M. Malagoli and R. Zanasi, Computational approach to molecular magnetic properties by continuous transformation of the origin of the current density 220 (1994) 299
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- Leahy, D.J., D.R. Cyr, D.L. Osborn and D.M. Neumark, Observation of the correlated  $O\ ^3P_{j1},\ ^3P_{j2}$  state distribution from the predissociation of  $O_2\ B\ ^3\Sigma_u^-$  216 (1993) 503
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- Lee, T.J., A coupled-cluster study of  $HNO_2$  and  $FNO_2$  216 (1993) 194
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- Lee, Y.R., C.L. Chiu and S.M. Lin, Photodissociation of  $S_2Cl_2$  at 308 nm by translational spectroscopy 216 (1993) 209

- Lee, Y.T., see D.W. Boo 211 (1993) 358
- Leegwater, J.A. and S. Mukamel, Four-wave mixing signatures of exciton Bose condensation 217 (1994) 456
- Legay, F. and N. Legay-Sommaire, NO diffusion and dimer formation in a nitrogen matrix studied by FTIR spectroscopy 211 (1993) 516
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- Legay-Sommaire, N., see F. Legay 211 (1993) 516
- Legay-Sommaire, N. and F. Legay, Photochemical formation of  $\text{CH}_3\text{HgH}$  in  $\text{Hg}/\text{CH}_4/\text{Ar}$  matrices studied by FTIR spectroscopy 217 (1994) 97
- Legon, A.C. and J.C. Thorn, Equilibrium nuclear quadrupole coupling constants from the rotational spectrum of  $\text{BrCl}$ : a source of the electric quadrupole moment ratios  $Q(^{79}\text{Br})/Q(^{81}\text{Br})$  and  $Q(^{35}\text{Cl})/Q(^{37}\text{Cl})$  215 (1993) 554
- Leininger, T., J.-F. Riehl, G.-H. Jeung and M. Péliissier, Reply to Comment on "Comparison of the widely used HF pseudo-potentials:  $\text{MH}^+$  ( $\text{M}=\text{Fe}, \text{Ru}, \text{Os}$ )" 220 (1994) 345
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- Lenderink, E., K. Duppen and D.A. Wiersma, Femtochemistry of the iodine-arene charge-transfer complex 211 (1993) 503
- Lenderink, E. and D.A. Wiersma, Photodissociation dynamics of dimethylnitrosamine studied by resonance Raman spectroscopy 218 (1994) 586
- Leone, S.R., see S.D. Price 214 (1993) 553
- Lequan, M., R.M. Lequan, K.C. Ching, M. Barzoukas, A. Fort, G. Bravic, D. Chasseau, Y. Barrans and M. Huché, Quadratic non-linear optical properties of N-(4-nitrostilbenyl) (S) prolinol 213 (1993) 71
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- Li, R.-J., K.-L. Han, F.-E. Li, R.-C. Lu, G.-Z. He and N.-Q. Lou, Rotational alignment of product molecules from the reactions  $\text{Sr} + \text{CH}_3\text{Br}$ ,  $\text{C}_2\text{H}_5\text{Br}$ ,  $n\text{-C}_3\text{H}_7\text{Br}$ ,  $i\text{-C}_3\text{H}_7\text{Br}$  by means of PLIF 220 (1994) 281



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- Li, Y., M. Honigmann, G. Hirsch and R.J. Buenker, Theoretical study of line broadening in the  $(3s\sigma)^3\Pi_g$  vibrational levels of the  $O_2$  molecule employing a diabatic CI representation 212 (1993) 185
- Li, Z., see J.S. Francisco 214 (1993) 77, 591
- Li, Z., A. Borrmann and C.C. Martens, Wavelet analysis of condensed phase molecular dynamics 214 (1993) 362
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- Li, Z., see R. Liu 219 (1994) 143
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- Liao, D.-W. and K. Balasubramanian, Germanium monochloride (GeCl). Spectroscopic constants and potential energy curves 213 (1993) 174
- Lichanot, A. and M. Rerat, Elastic properties in BeO. An ab initio Hartree-Fock calculation 211 (1993) 249
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- Liebermann, H.-P., I. Boustani, S.N. Rai, A.B. Alekseyev, G. Hirsch and R.J. Buenker, Use of relativistic core potentials to compute potential curves and lifetimes of low-lying states of arsenic fluoride 214 (1993) 381
- Lienau, Ch., J.C. Williamson and A.H. Zewail, Femtochemistry at high pressures. The dynamics of an elementary reaction in the gas-liquid transition region 213 (1993) 289
- Light, J.C., see D.E. Manolopoulos 216 (1993) 18
- Lim, E.C., see H. Saigusa 211 (1993) 410
- Lim, S.K., M.E. Burba and A.C. Albrecht, The Stokes law radius of the  $C_{60}$  radical anion in *n*-hexane by time-of-flight mobility measurements 216 (1993) 405
- Lin, S.H., see M. Hayashi 213 (1993) 465
- Lin, S.H., see B. Fain 216 (1993) 551
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- Lin, Z., K. Boraas and J.P. Reilly, The vibrational overtone spectrum of fluoroform in the  $\Delta\nu=4$  C-H stretching region 217 (1994) 239
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- Liu, F., S.H. Garofalini, R.D. King-Smith and D. Vanderbilt, Structural and electronic properties of sodium metasilicate 215 (1993) 401
- Liu, K., see Z. Ma 213 (1993) 269
- Liu, L., see H. Guo 218 (1994) 212
- Liu, R. and X. Zhou, Comment on "Cyclopentadienylideneketene: theoretical confirmation of a key infrared band" 212 (1993) 702
- Liu, R., S. Ma and Z. Li, Theoretical study on the dynamic properties and state-selected rate constants of the reaction  $CH(^4\Sigma^-) + H_2 \rightarrow CH_2(^3B_1) + H$  219 (1994) 143
- Liu, X.-Y., P. Bennema, L.A. Meijer and M.S. Couto, Ordering of paraffin-like molecules at the solid-fluid interface 220 (1994) 53
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- Liu, Z., see P.B. Davies 214 (1993) 305
- Liyanage, R., P.T.A. Reilly, Y. Yang, R.J. Gordon and R.W. Field, Evidence of the indirect predissociation of the  $F^1\Delta$  state of HCl 216 (1993) 544

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- Loo, B.H., Enhanced Raman scattering from hexacyanoferrate (II) and (III) ions adsorbed on silver electrode surfaces 213 (1993) 479
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- Lüchow, A., see H. Kleindienst 218 (1994) 441
- Luckhaus, D., M. Quack and J. Stohner, Femtosecond quantum structure, equilibration and time reversal for the CH-chromophore dynamics in  $\text{CHD}_2\text{F}$  212 (1993) 434
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- Luo, Y., H. Ågren, S. Knuts and P. Jørgensen, The two-photon spectrum of pyrimidine. Role of vibronic coupling 213 (1993) 356
- Lynch, G.C., see S.L. Mielke 213 (1993) 10; 216 (1993) 441; 217 (1994) 173
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- Ma, N.L., S.S. Wong, M.N. Paddon-Row and W.-K. Li, Is HPC a minimum on the HCP potential surface? A failure of the Møller-Plesset perturbation theory 213 (1993) 189
- Ma, N.L., see Z.-X. Ma 213 (1993) 250
- Ma, S., see R. Liu 219 (1994) 143
- Ma, X., see Y. Chen 211 (1993) 449
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- Ma, Z. and K. Liu, Collision-induced fine-structure transition of  $O(^3P_2) \rightarrow O(^3P_{1,0})$  by He and  $H_2$ : excitation function and branching ratio 213 (1993) 269
- Ma, Z.-X., C.-L. Liao, H.-M. Yin, C.Y. Ng, S.-W. Chiu, N.L. Ma and W.-K. Li, Experimental and theoretical studies of isomeric  $C_2H_5S$  and  $C_2H_5S^+$  213 (1993) 250
- Maas, W.E., see D.G. Cory 212 (1993) 487
- Mac, M. and J. Wirz, Deriving intrinsic electron-transfer rates from nonlinear Stern-Volmer dependencies for fluorescence quenching of aromatic molecules by inorganic anions in acetonitrile 211 (1993) 20
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- Mafuné, F., J. Kohno, T. Nagata and T. Kondow, Mechanism of ion ejection from a liquid beam following laser photoionization 218 (1994) 7
- Mafuné, F., Y. Takeda, T. Nagata and T. Kondow, Inhomogeneous solvation in an aniline-ethanol solution studied by laser photoionization of a liquid beam 218 (1994) 234
- Magnasco, V., A. Siciliano and G. Figari, Variationally improving the Inui wavefunction for  $H_2$  213 (1993) 17
- Magnera, T.F., D.M. Sammond and J. Michl, Ground-state rotational constants of  $Ar_3^+$  by rotational depletion coherence spectroscopy 211 (1993) 378
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- Mahi, L., J.C. Duplan and B. Fenet, Suppression of  $J$ -modulation effects for resonance editing by NMR spin-echo experiments 211 (1993) 27
- Mai, J., A. Casties and W. von Niessen, A Monte Carlo simulation for the catalytic oxidation of CO on DLA clusters 211 (1993) 197
- Maier, J.P., see M. Fehér 211 (1993) 171
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- Maluendes, S.A., A.D. McLean and E. Herbst, New calculations on the ion-molecule processes  $C_2H_2^+ + H_2 \rightarrow C_2H_3^+ + H$  and  $C_2H_2^+ + H_2 \rightarrow C_2H_4^+$  217 (1994) 571



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- Manolopoulos, D.E. and J.C. Light, A log derivative formulation of reaction rate theory 216 (1993) 18
- Mansfeld, M. and W.S. Veeman, The use of  $^{129}\text{Xe}$  NMR exchange spectroscopy for probing the microstructure of porous materials 213 (1993) 153
- Manthe, U. and A.D. Hammerich, Wavepacket dynamics in five dimensions. Photodissociation of methyl iodide 211 (1993) 7
- Mao, X., J. Guo and C. Ye, Competition between radiation damping and transverse relaxation effects on NMR signal intensities 218 (1994) 249
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- Marconi, G., see G. Giro 211 (1993) 580
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- Mares, J.A., G. Boulon, A. Brenier, L. Lou and S.R. Rotman, Spectroscopy of multisites  $\text{Cr}^{3+}$  and  $\text{Nd}^{3+}$  in yttrium aluminum perovskite 217 (1994) 105
- Maresch, G.G., see M. Hubrich 218 (1994) 81
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- Maricq, M.M. and J.J. Szente, Upper limits for the rate constants of the reactions  $\text{CF}_3\text{O} + \text{O}_3 \rightarrow \text{CF}_3\text{O}_2 + \text{O}_2$  and  $\text{CF}_3\text{O}_2 + \text{O}_3 \rightarrow \text{CF}_3\text{O} + 2\text{O}_2$  213 (1993) 449
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- Martrenchard-Barra, S., C. Jouvet, C. Lardeux-Dedonder and D. Solgadi, Molecular dynamics simulations of the formation process of very small doubly charged para-difluorobenzene clusters produced in a supersonic expansion 215 (1993) 291
- Maruyama, K., see A. Osuka 215 (1993) 179
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- Masaki, A., S. Tsunashima and N. Washida, Rate constant for the reaction of  $\text{CH}_3\text{O}_2$  with NO 218 (1994) 523
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- Matsuoka, O., Reply to Comment on "Segmented contractions of relativistic Gaussian basis sets" 212 (1993) 550
- Matsushita, M., A.M. Frens, E.J.J. Groenen, O.G. Poluektov, J. Schmidt, G. Meijer and M.A. Verheijen, Triplet excitations of crystalline C<sub>60</sub>. An optically detected magnetic-resonance study in zero field 214 (1993) 349
- Matsuzaki, S.Y., see S. Murata 219 (1994) 200
- Matsuzaki, Y., K. Tanaka and T. Yamabe, Electronic excitations to higher two-photon states of conjugated polymers 211 (1993) 300
- Mattar, S.M. and B.J. Doleman, MRSD-CI and LDF studies of the VN X <sup>3</sup>Δ and D <sup>3</sup>Π states 216 (1993) 369
- Matveets, Yu.A., see I.V. Bezel 218 (1994) 475
- Matveev, A.A., A.M. Pravilov and A.F. Vilesov, Anomalous large isotope effect in the chemiluminescence from N(<sup>4</sup>S) + O(<sup>3</sup>P) recombination 217 (1994) 582
- Matyushov, D.V. and R. Schmid, Stationary points in the temperature dependence of electron transfer rates 220 (1994) 359
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- McCormack, E.F., S.T. Pratt, P.M. Dehmer and J.L. Dehmer, Double-resonance laser-induced grating spectroscopy of nitric oxide 211 (1993) 147
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- McGibbon, G.A., P.C. Burgers and J.K. Terlouw, O-protonated sulfine CH<sub>2</sub>=S=OH<sup>+</sup>. Its generation from ionized dimethylsulfoxide by delayed dissociation 218 (1994) 499

- McGlynn, S.P., see U. Asaf 212 (1993) 326
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- McKee, M.L., Theoretical study of the  $\text{CH}_3\text{SOO}$  radical 211 (1993) 643
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- McLauchlan, K.A., see S.N. Batchelor 214 (1993) 507
- McLauchlan, K.A., I.A. Shkrob and M.T. Yeung, Room-temperature observations of spin-polarized triplet anthracene 217 (1994) 157
- McLean, A.D., see S.A. Maluendes 217 (1994) 571
- McLuckey, S.A., see L.D. Hulett Jr. 216 (1993) 236
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- Mebel, A.M., D.G. Musaev and K. Morokuma, Ab initio molecular orbital study of structure and NMR  $^{11}\text{B}$  chemical shifts of Lewis base adducts of  $\text{CO}$ ,  $\text{NH}_3$ ,  $\text{PF}_3$ , and  $\text{PH}_3$  with small nido-boranes,  $\text{B}_3\text{H}_7$  and  $\text{B}_4\text{H}_8$  214 (1993) 69
- Mebel, A.M., D.G. Musaev and K. Morokuma, An alternative mechanism of  $\text{BH}_2\text{SH}$  formation in the reaction of  $\text{B}_2\text{H}_6$  with  $\text{SH}_2$ : concerted elimination of  $\text{BH}_3$  and  $\text{H}_2$  from  $\text{H}_2\text{S}\cdot\text{B}_2\text{H}_6$ . Ab initio MO study 216 (1993) 313
- Medikeri, M.N. and M.K. Mishra, Quasiparticle approximation to the dilated electron propagator with application to  $^2\text{P}$  shape resonances in e-Be and e-Ca scattering 211 (1993) 607
- Medina, A., see J.M.M. Roco 216 (1993) 593
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- Meier, Ch. and V. Engel, Electron kinetic energy distributions from multiphoton ionization of  $\text{Na}_2$  with femtosecond laser pulses 212 (1993) 691
- Meijer, G., see M. Matsushita 214 (1993) 349
- Meijer, G., see M.A. Verheijen 216 (1993) 72
- Meijer, G., M.G.H. Boogaarts, R.T. Jongma, D.H. Parker and A.M. Wodtke, Coherent cavity ring down spectroscopy 217 (1994) 112
- Meijer, G., see J.L. de Boer 219 (1994) 469
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- Meissner, L., A. Balková and R.J. Bartlett, Multiple solutions of the single-reference coupled-cluster method 212 (1993) 177
- Meller, J., J.L. Heully and J.P. Malrieu, Size-consistent self-consistent combination of selected CI and perturbation theory 218 (1994) 276
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- Menon, M. and K.R. Subbaswamy, Structure of  $\text{Si}_{60}$ . Cage versus network structures 219 (1994) 219
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- Meskers, S.C.J., J.P. Riehl and H.P.J.M. Dekkers, Linearly polarized luminescence spectra of  $\text{Eu}(\text{2,6-pyridine-dicarboxylate})_3^{3-}$  in hydroxylic solution 216 (1993) 241
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- Mestechkin, M.M. and G.E. Whyman, Time-dependent Hartree-Fock theory: finite-field technique for calculation of the Pockels and Kerr effects and generation of harmonics 214 (1993) 144
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- Mhin, B.J., J. Kim and K.S. Kim, Entropy-driven structures of the hexaaqua-sodium(I) 216 (1993) 305
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- Mielke, S.L., G.C. Lynch, D.G. Truhlar and D.W. Schwenke, A more accurate potential energy surface and quantum mechanical cross section calculations for the  $F + H_2$  reaction 213 (1993) 10
- Mielke, S.L., G.C. Lynch, D.G. Truhlar and D.W. Schwenke, A separable rotation approximation for the calculation of chemical reaction rates 216 (1993) 441
- Mielke, S.L., G.C. Lynch, D.G. Truhlar and D.W. Schwenke, A more accurate potential energy surface and quantum mechanical cross section calculations for the  $F + H_2$  reaction (Chem. Phys. Letters 213 (1993) 10). Erratum 217 (1994) 173
- Miguel, B., see J.M. García de la Vega 212 (1993) 420
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- Miki, H., S. Kimachi, R. Satomi, T. Azumi and M. Onishi, Zero-field splittings of the ligand localized  $^3\pi\pi^*$  phosphorescence of the Ru(II) complex with the  $\pi$ -conjugated ligand 218 (1994) 563
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- Mimuro, M., Y. Nishimura, S. Takaichi, Y. Yamano, M. Ito, S. Nagaoka, I. Yamazaki, T. Katoh and U. Nagashima, The effect of molecular structure on the relaxation processes of carotenoids containing a carbonyl group 213 (1993) 576
- Minaev, B. and H. Ågren, The interpretation of the Wulf absorption band of ozone 217 (1994) 531
- Ming, L., S. Nordholm, G. Nyman and J. Davidsson, Monte Carlo simulation study of statistical limits for energy transfer in binary molecular collisions 211 (1993) 189
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- Miyajima, S., A.F. McDowell and R.M. Cottis, Pulsed-field-gradient stimulated-spin-echo NMR study of anisotropic self-diffusion in smectic Ad liquid crystal CBOOA 212 (1993) 277
- Miyatake, Y., see H. Hase 215 (1993) 141
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- Miyazaki, T., K. Yamamoto and J. Arai, Effect of rotational quantum states ( $J=0, 1$ ) of matrix  $H_2$  molecules on ESR spectra of radicals at 4.2 K 219 (1994) 405
- Miyazaki, Y., T. Matsuo and H. Suga, Glass transition of myoglobin crystal 213 (1993) 303
- Mizuki, J., see K. Tanigaki 213 (1993) 395
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- Mó, O., M. Yáñez, I. Rozas and J. Elguero, Structure, vibrational frequencies and thermodynamic properties of hydrogen peroxide-water dimers. An ab initio molecular orbital study 219 (1994) 45
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- Mohan, H., D.K. Maity and J.P. Mittal, Effect of fluorine substitution on the  $\cdot OH$ -radical-induced electron-transfer reaction in aqueous solutions of fluorinated alkyl iodides 220 (1994) 455
- Moine, B., see C. Pédrini 220 (1994) 433
- Molin, Yu.N. and K.M. Salikhov, Spin exchange interaction as a possible source of oscillations in recombination of spin-correlated radical pairs 211 (1993) 484
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- Momigny, J. and R. Loch, The appearance of  $C_2H_3^+$  ions from  $C_2H_3F$  by non-resonant photoionization. A translational energy surprisal analysis 211 (1993) 161
- Monks, P.S., L.J. Stief, M. Krauss, S.C. Kuo and R.B. Klemm, A discharge-flow photoionization mass-spectrometric study of the  $BrO(X^2\Pi)$  radical. Photoionization spectrum and ionization energy 211 (1993) 416
- Montgomery Jr., J.A., H.H. Michels and J.S. Francisco, Ab initio calculation of the heats of formation of  $CF_3OH$  and  $CF_2O$  220 (1994) 391
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- Mori, Y., Y. Nakamichi, T. Sekiguchi, N. Okazaki, T. Matsumura and I. Hanazaki, Photoinduction of chemical oscillation in the Belousov-Zhabotinsky reaction under the flow condition 211 (1993) 421
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- Morley, G.P., P. Felder and J.R. Huber, Photodissociation of dichlorocarbene  $\text{CCl}_2$  at 248 nm in a cold beam 219 (1994) 195
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- Morris, V.R., F. Mohammad, L. Valdry and W.M. Jackson, Steric effects on nascent vibrational distributions of the HCN product produced in CN radical reactions with ethane, propane and chloroform 220 (1994) 448
- Morse, M.D., see J.C. Pinegar 212 (1993) 458
- Morton, J.R., F. Negri and K.F. Preston, The EPR spectra of hydrides of  $\text{C}_{70}$ . An experimental and theoretical investigation 218 (1994) 467
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- Motyakin, M.V. and N.G. Spitchina, ESR study of the fullerene  $\text{C}_{60}$  under axial and shear deformation 216 (1993) 63
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- Mukai, K., K. Nedachi, J.B. Jamali and N. Achiwa, Magnetic properties of 1,5-dimethylverdazyl radicals. I. Evidence for the ferromagnetic exchange interaction in 3-(4-chlorophenyl)-1,5-dimethyl-6-thioxoverdazyl radical solid 214 (1993) 559
- Mukai, M., see Y. Fujiwara 213 (1993) 89
- Mukaihata, H., T. Ohkubo, Y. Fujiwara and M. Itoh, Picosecond time-resolved fluorescence of the intramolecular excited-state proton transfer in 2-naphthyl-3-hydroxychromones. Torsional relaxation in the excited states 211 (1993) 140
- Mukamel, S., see A. Takahashi 216 (1993) 394
- Mukamel, S., see J.A. Leegwater 217 (1994) 456
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- Murata, S., M. Nishimura, S.Y. Matsuzaki and M. Tachiya, Transient effect in fluorescence quenching induced by electron transfer. I. Analysis by the Collins-Kimball model of diffusion-controlled reactions 219 (1994) 200
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- Nagalakshmi, V., V. Lakshminarayana, G. Sumithra and M. Durga Prasad, Coupled cluster description of anharmonic molecular vibrations. Application to  $O_3$  and  $SO_2$  217 (1994) 279
- Nagaminé, M., see T. Tsukuda 218 (1994) 1
- Nagano, Y., T. Kiyobayashi and T. Nitta,  $CO_2$  absorption in  $C_{60}$  solid 217 (1994) 186
- Naganuma, T., see K. Hoshino 211 (1993) 571
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- Nagao, H., K. Nishikawa and S. Aono, The Hückel model by means of the path integral method. II. Application to the square lattice system 215 (1993) 5
- Nagaoka, S., see M. Mimuro 213 (1993) 576
- Nagase, S. and K. Kobayashi, Metallofullerenes  $MC_{82}$  ( $M=Sc, Y$ , and  $La$ ). A theoretical study of the electronic and structural aspects 214 (1993) 57
- Nagashima, U., see M. Mimuro 213 (1993) 576
- Nagata, T., see T. Tsukuda 218 (1994) 1
- Nagata, T., see F. Mafuné 218 (1994) 7, 234
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- Nagy, G. and D. Roy, Surface charge dependence of second harmonic generation from a Ni electrode 214 (1993) 197
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- Naik, P.D., see S. Koppe 214 (1993) 546
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- Nakai, T. and C.A. McDowell, Residual chemical-shift effects in spin-echo NMR powder patterns of homonuclear dipolar-coupled spins 217 (1994) 234
- Nakajima, A., see K. Hoshino 211 (1993) 571
- Nakajima, A., T. Taguwa, K. Hoshino, T. Sugioka, T. Naganuma, F. Ono, K. Watanabe, K. Nakao, Y. Konishi, R. Kishi and K. Kaya, Photoelectron spectroscopy of  $(C_6F_6)^-$  and  $(Au-C_6F_6)^-$  clusters 214 (1993) 22
- Nakajima, T., see H. Sekiya 215 (1993) 499
- Nakamatsu, H., see J. Onoe 217 (1994) 61
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- Nakamura, Y., M. Igarashi, Y. Sakaguchi and H. Hayashi, Effects of high magnetic fields on the dynamic behavior of radical pairs generated in micellar solutions 217 (1994) 387
- Nakao, K., see A. Nakajima 214 (1993) 22
- Nakao, Y., see K. Kikuchi 216 (1993) 67
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- Nakayama, T., C. Honma, S. Miki and K. Hamanoue, Intra- and inter-molecular hydrogen-atom abstraction of photoexcited 1,4-dimethylantraquinone 213 (1993) 581

- Nakayama, T., T. Takahashi, K. Ibuki and K. Hamanoue, Intracomplex electron transfer upon direct excitation of a ground-state complex of benzophenone with 2,5-dimethyl-2,4-hexadiene 215 (1993) 622
- Nakayama, T., S. Miki, F.M. Abdel-Latif, K. Ibuki and K. Hamanoue, Spectroscopic study of the formation and decay of intermediates for the novel photochemistry of sterically strained [6]-1,4-cyclophaneanthraquinone 220 (1994) 219
- Nanayakkara, A., see J. Cioslowski 219 (1994) 151
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- Negri, F., G. Orlandi, F. Zerbetto, G. Ruani, A. Zakhidov, C. Taliani, K. Kinuchi and Y. Achiba, Scattering of the vibrational frequencies of <sup>13</sup>C<sub>x<sup>12</sup>C<sub>60-x</sub>. A Raman spectroscopy and quantum chemical study 211 (1993) 353</sub>
- Negri, F., see J.R. Morton 218 (1994) 467
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- Nemes, L., R.S. Ram, P.F. Bernath, F.A. Tinker, M.C. Zumwalt, L.D. Lamb and D.R. Huffman, Gas-phase infrared emission spectra of C<sub>60</sub> and C<sub>70</sub>. Temperature-dependent studies 218 (1994) 295
- Nemeth, G.I., H.L. Selzle and E.W. Schlag, Magnetic ZEKE experiments with mass analysis 215 (1993) 151
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- Neugebauer, S.M. and D.S. Tinti, Deuterium isotope effects on the zero-field splittings of the lowest triplet state of benzaldehyde derivatives 211 (1993) 555
- Neumann, B., Zs. Nagy-Ungvarai and S.C. Müller, Interaction between silica gel matrices and the Belousov-Zhabotinsky reaction 211 (1993) 36
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- Nguyen Vien, G., N. Rougeau and C. Kubach, H-atom exchange in low energy IH( $\nu=0$ ) + I collisions. Effect of the potential energy surface 215 (1993) 35
- Nicholson, D., see A. Boutin 219 (1994) 484
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- Nicolaides, C.A., T. Mercouris and I.D. Petsalakis, Above and below threshold multipho-ton dissociation of volcanic ground states. Application to BeH 212 (1993) 685
- Nicolaisen, H.-W., see H. Harder 214 (1993) 265
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- Nielsen, O.J. and J. Sehested, Upper limits for the rate constants of the reactions of CF<sub>3</sub>O<sub>2</sub> and CF<sub>3</sub>O radicals with ozone at 295 K 213 (1993) 433



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 Nobusada, K., K. Sakimoto and K. Onda, Quantum mechanical close coupling calculations of collision-induced dissociation in  $\text{He} + \text{H}_2$ . A discretized continuum model 216 (1993) 613  
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- Nunzi, J.-M., F. Charra, C. Fiorini and J. Zyss, Transient optically induced non-centro-symmetry in a solution of octupolar molecules 219 (1994) 349
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Ohshima, Y. and Y. Endo, Fourier-transform microwave spectroscopy of <sup>24</sup>Mg<sup>35</sup>Cl generated by laser ablation 213 (1993) 95  
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O'Malley, P.J., H. Soscun and S.J. Collins, The "true" minimum energy structure of H<sub>3</sub>SiOHAlH<sub>3</sub>. Implications for conformational preferences of bridged hydroxyl groups in zeolites 217 (1994) 293  
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- Onoe, J., R. Sekine, K. Takeuchi, H. Nakamatsu, T. Mukoyama and H. Adachi, Atomic-number dependence of relativistic effects on chemical bonding using the non-relativistic and relativistic discrete-variational  $X\alpha$  methods 217 (1994) 61
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- Ottinger, Ch. and A.F. Vilesov, LIF detection of the  $A' \ ^5\Sigma_g^+$  state of  $N_2$  in a beam and lifetime of the  $C'' \ ^5\Pi_u$  state 211 (1993) 175
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- Pan, X. and R.A. MacPhail, A Raman study of cyclopentane- $d_9$  pseudorotation dynamics as a function of pressure 212 (1993) 64
- Panas, I., Structures of some hydrogen-bonded molecular clusters from ab initio hard-spheres electrostatics 216 (1993) 173
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- Papakondylis, A. and A. Mavridis, Electronic and geometrical structure of the  $\text{NF}_2$  radical 216 (1993) 167
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- Park, I.J. and S.I. Woo, Computer simulation of spatial coupling in chemical oscillations of CO oxidation on two Pd(110) single crystals 212 (1993) 505
- Park, J. and J.F. Hershberger, Kinetics of  $\text{NCO} + \text{hydrocarbon}$  reactions 218 (1994) 537
- Park, J.K. and H. Sun, Dipole moment functions of  $\text{NH}$  and  $\text{NH}^+$  by ab initio effective valence shell Hamiltonian 211 (1993) 618
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- Parmigiani, F. and L. Sangaletti, Electronic correlation effects in the Ni 3s and Co 3s X-ray photoelectron spectra of  $\text{NiO}$ ,  $\text{CoO}$ ,  $\text{K}_2\text{NiF}_4$  and  $\text{K}_2\text{CoF}_4$  213 (1993) 613
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- Peel, J.B., Configuration interaction calculations of the structure and energetics of the high symmetry isomers of the  $\text{O}_4^+$  cation 218 (1994) 367
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- Petersen, B.L., L.J. Terminello, J.J. Barton and D.A. Shirley, Photoelectron holography of Pt(111) at 351 eV 213 (1993) 412
- Petersen, B.L., L.J. Terminello, J.J. Barton and D.A. Shirley, Multiple-wavenumber photoelectron holography of Pt(111) 220 (1994) 46
- Petrella, G. and L. Cassidei, Atom scattering from disordered surfaces. Theoretical study on the validity of the cross section overlap hypothesis: the case of vacancies on Pt(111) 212 (1993) 512
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- Rabinowitz, M., Phenomenological theory for short coherence length superconductivity 216 (1993) 571
- Rabinowitz, M. and T. McMullen, General model of pressure-induced transition temperature increase with focus on the Hg-Ba-Ca-Cu-O system 218 (1994) 437
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- Raghavachari, K., B. Zhang, J.A. Pople, B.G. Johnson and P.M.W. Gill, Isomers of C<sub>24</sub>. Density functional studies including gradient corrections 220 (1994) 385
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- Ramiro Diaz, B., P. Wahnö and V. Sidis, A calculated (KrO<sub>2</sub>)<sup>+</sup> ground-state potential energy surface 212 (1993) 218
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- Rashev, S., A theoretical study of internal conversion in benzene 217 (1994) 69
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- Ravichandran, K., R. Williams and T.R. Fletcher, Atmospheric reactions of vibrationally excited greenhouse gases: SH + N<sub>2</sub>O(*n*, 0, 0) 217 (1994) 375
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- Reis e Sousa, A.T., E.M.S. Castanheira, J.M.G. Martinho, S. Saghbini, F. Baros, J.C. André and M.A. Winnik, Influence of pressure on cyclization of a polystyrene chain. Time-resolved fluorescence measurements 213 (1993) 333
- Reisfeld, R., see R. Gvishi 212 (1993) 463; 213 (1993) 338
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- Remita, S., J.M. Orts, J.M. Feliu, M. Mostafavi and M.O. Delcourt, STM identification of silver oligomer clusters prepared by radiolysis in aqueous solution 218 (1994) 115
- Remmers, G., M. Domke, A. Puschmann, T. Mandel, G. Kaindl, E. Hudson and D.A. Shirley, High-resolution inner-shell photoionization of NO 214 (1993) 241
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- Ribeiro, S.J.L., R.E.O. Diniz, Y. Messaddeq, L.A. Nunes and M.A. Aegerter,  $\text{Eu}^{3+}$  and  $\text{Gd}^{3+}$  spectroscopy in fluoroindate glasses 220 (1994) 214
- Ribeiro-Claro, P.J.A., see R.D. Gordon 211 (1993) 392
- Ricciardi, G., F. Lelj and F. Bonosi, Synthesis and physico-chemical properties of the bis(2,3,7,8,12,13,17,18-octakis-(octylthio)-5,10,15,20-tetraazaporphyrinato)-lutetium(III) complex 215 (1993) 541
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- Riesen, H., E. Krausz and L. Dubicki, Probing the distribution of low symmetry fields by the magnetic field effect on a persistent spectral hole in the  $R_1$  line of chromium(III)-tris(2,2'-bipyridine) in glycerol 218 (1994) 579
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- Schlütter, J., R. Schott and K. Kleinermanns, State selective investigation of the reactions  $O(^1D) + CH_4$  ( $C_2H_6$ )  $\rightarrow$  OH ( $CH_2OH$ ) +  $CH_3(\nu_1(\nu), \nu_2(\nu), J, K)$  using resonant multiphoton ionization detection of  $CH_3$  213 (1993) 262
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- Schroeder, J., D. Schwarzer, J. Troe and P. Vöhringer, From barrier crossing to barrierless relaxation dynamics. Photoisomerization of trans-stilbene in compressed *n*-alkanols 218 (1994) 43
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- Scott, A.P. and L. Radom, Reply to Comment on "Cyclopentadienylideneketene: theoretical confirmation of a key infrared band" 212 (1993) 705
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- Sekiya, H., T. Nakajima, H. Ujita, T. Tsuji, S. Ito and Y. Nishimura, Proton tunneling in tropolone-Rg (Rg=Ar, Kr, Xe) van der Waals complexes 215 (1993) 499
- Sekiya, H., M. Habu, H. Ujita, T. Tsuji, A. Mori, H. Takeshita, Y. Nishimura, H. Petek and K. Yoshihara, Dual fluorescence and excited-state intramolecular proton transfer in jet-cooled 3,4-benzotropolone 215 (1993) 641
- Sekkat, Z., M. Büchel, H. Orendi, H. Menzel and W. Knoll, Photoinduced alignment of azobenzene moieties in the side chains of polyglutamate films 220 (1994) 497
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- Simpson, W.R., A.J. Orr-Ewing and R.N. Zare, State-to-state differential cross sections for the reaction  $\text{Cl}(^2\text{P}_{3/2}) + \text{CH}_4(\nu_3 = 1, J = 1) \rightarrow \text{HCl}(\nu' = 1, J') + \text{CH}_3$  212 (1993) 163
- Sims, I.R., J.-L. Queffelec, D. Travers, B.R. Rowe, L.B. Herbert, J. Karthäuser and I.W.M. Smith, Rate constants for the reactions of CN with hydrocarbons at low and ultra-low temperatures 211 (1993) 461  
220 (1994) 203
- Singh, A.K., see S.K. Ramasesha
- Singh, R.K., B.P. Asthana and H.D. Bist, Study of the dynamics of phase transition in  $\text{NH}_4\text{SCN}$  by a precise Raman linewidth and frequency shift measurement (Chem. Phys. Letters 209 (1993) 390). Erratum 213 (1993) 210
- Singleton, S.M. and R.D. Coombe, Rate and mechanism of the  $\text{NH}(a^1\Delta) + \text{Cl}_2$  reaction 215 (1993) 237
- Sinha, A., see D.E. Govoni 216 (1993) 525
- Sinha, H.K. and R.P. Steer,  $\text{S}_2\text{-S}_0$  fluorescence excitation spectroscopy of van der Waals complexes of xanthione and benzopyranthione with  $\text{N}_2$  and CO 211 (1993) 397
- Siska, P.E., see M.F. Falcetta 213 (1993) 531
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- Skiebe, A., A. Hirsch, H. Klos and B. Gotschy,  $[\text{DBU}]\text{C}_{60}$ . Spin pairing in a fullerene salt 220 (1994) 138
- Skourtis, S.S. and J.N. Onuchic, Effective two-state systems in bridge-mediated electron transfer. A Green function analysis (Chem. Phys. Letters 209 (1993) 171). Erratum 211 (1993) 282
- Skurat, V.E., see A.P. Nikiforov 212 (1993) 43
- Smeyers, Y.G., see V. Botella 219 (1994) 497
- Smirnov, S.N. and C.L. Braun, Light polarization effects in the transient dc conductivity response to excitation of dipolar solutes 217 (1994) 167
- Smirnov, V.V., see M. Ehbrecht 214 (1993) 34
- Smit, T.S. and K.H. Johnson, Hydrodesulphurization of thiophene by transition metal sulphides. A molecular orbital topology study 212 (1993) 525
- Smith, D. and P. Španel, Dissociative recombination of  $\text{H}_3^+$ . Experiment and theory reconciled 211 (1993) 454
- Smith, D., P. Španel and T.D. Märk, Electron attachment to  $\text{C}_{60}$  at low energies 213 (1993) 202

- Smith, D.M., R.P. Tuckett, K.R. Yoxall, K. Codling and P.A. Hatherly, Fragmentation of the  $\tilde{C}^2T_2$  and  $\tilde{D}^2A_1$  states of  $CCl_4^+$  and  $SiCl_4^+$  studied by threshold photoelectron-photoion coincidence spectroscopy 216 (1993) 493
- Smith, I.W.M., see I.R. Sims 211 (1993) 461
- Smith, M.E., C. Jaeger, R. Schoenhofer and S. Steuernagel, Structural characterisation of the aluminium sites in kyanite by  $^{27}Al$  magic angle spinning centreband, satellite transition and double rotation NMR 219 (1994) 75
- Smith, P.E. and W.F. Van Gunsteren, The viscosity of SPC and SPC/E water at 277 and 300 K 215 (1993) 315
- Smith, P.G., see T. Troxler 211 (1993) 371
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- Smith Jr., V.H., see J. Wang 220 (1994) 331
- Snyder, G. and D. Sapse, Ab initio studies of complexes of ozone with some positive ions 218 (1994) 372
- Sobolewski, A.L. and W. Domcke, Evidence for the need of a non-Born–Oppenheimer description of excited-state hydrogen transfer 211 (1993) 82
- Sobolewski, A.L., The mechanism of excited-state hydrogen transfer in 2-hydroxypyridine 211 (1993) 293
- Sodupe, M. and C.W. Bauschlicher Jr., A theoretical study of the spectroscopy of  $SrH_2O^+$  and  $SrNH_3^+$  212 (1993) 624
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- Song, X., Y. Bao, R.S. Urdahl, J.N. Gosine and W.M. Jackson, Laser-induced fluorescence studies of  $C_3$  formation and isomerization in the 193 nm photolysis of allene and propyne 217 (1994) 216
- Song, Z., R. Lu, N. Lou and R. Zhai, The effect of exchange process on the kinetics of desorption and adsorption of CO on Rh(111) surface 217 (1994) 142
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- Sosa, C., C. Lee, G. Fitzgerald and R.A. Eades, Chemical applications of density functional theory:  $F_3^-$  anion dissociation ( $F_3^- \rightarrow F_2 + F^-$ ) 211 (1993) 265
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- Spano, F.C., Mean-field nonlinear optical susceptibility of charge-transfer crystals 211 (1993) 491
- Spano, F.C., Theory of strong-field pump–probe spectroscopy in J-aggregates 220 (1994) 365
- Spielfiedel, A., N. Feautrier, G. Chambaud, P. Rosmus and H.-J. Werner, The first dipole-allowed electronic transition  $1^1\Sigma_u^+ - X^1\Sigma_g^+$  of  $CO_2$  216 (1993) 162
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- Stahl, T., see H. Lanig 220 (1994) 423
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- Štich, I., M.C. Payne, A. De Vita, M.J. Gillan and L.J. Clarke, Chemically driven molecular decomposition at semiconductor surfaces 212 (1993) 617
- Stickel, R.E., Z. Zhao and P.H. Wine, Branching ratios for hydrogen transfer in the reactions of OD radicals with  $\text{CH}_3\text{SCH}_3$  and  $\text{CH}_3\text{SC}_2\text{H}_5$  212 (1993) 312
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- Stoeckel, F., see A. Charvát 214 (1993) 495
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- Strout, D.L., R.L. Murry, C. Xu, W.C. Eckhoff, G.K. Odom and G.E. Scuseria, A theoretical study of buckminsterfullerene reaction products:  $C_{60} + C_{60}$  214 (1993) 576
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- Stuhlmann, C., I. Villegas and M.J. Weaver, Scanning tunneling microscopy and infrared spectroscopy as combined in situ probes of electrochemical adlayer structure. Cyanide on Pt(111) 219 (1994) 319
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- Sun, H., see J.K. Park 211 (1993) 618
- Sun, W., G. Sha, B. Jiang, E.J. Hints and C. Zhang, *M*- and *e/f*-symmetry-resolved cross sections for  $CO(A^1\Pi)-He/Ar$  collision-induced energy transfer from  $J=2$  to  $J=1$  218 (1994) 515
- Sun, W., see G. Ding 220 (1994) 1
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- Sunderlin, L.S. and R.R. Squires, Determination of the  $H_2O-NO_2^+$  and  $CH_3O(H)-NO_2^+$  bond strengths and the proton affinities of nitric acid and methyl nitrate 212 (1993) 307
- Sundholm, D. and J. Olsen, Core-valence correlation effects on the ground state electron affinity of calcium 217 (1994) 451
- Sundqvist, B.U.R., see P.A. Brühwiler 214 (1993) 45
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- Supronowicz, J., M.J. Hinek, J.B. Atkinson and L. Krause, Mixing of the  $Cd\ 5^3P$  fine-structure states by Hg collisions 213 (1993) 282

- Supronowicz, J., E. Hegazi, J.B. Atkinson and L. Krause, Laser spectroscopy of some high-lying HgZn spin-orbit states 218 (1994) 240
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- Suter, D., see T. Blasberg 215 (1993) 668
- Suter, U.W., see M. Tomaselli 214 (1993) 1
- Suvernev, A.A. and T. Dreier, Evaluation of CARS spectra. Spectra of symmetric molecules in the Keilson-Storer model 216 (1993) 1
- Suvernev, A.A. and T. Dreier, Evaluation of CARS spectra. Doppler broadening in spectra of linear molecules 216 (1993) 5
- Suwaiyan, A., see K.A. Al-Hassan 212 (1993) 581
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- Swiech, W., see B. Rausenberger 215 (1993) 109
- Sworakowski, J., K. Palewska and M. Bertault, A calorimetric study of phase transitions in C<sub>70</sub> fullerene 220 (1994) 197
- Syage, J.A., Predissociation lifetimes of the  $\tilde{B}$  and  $\tilde{C}$  Rydberg states of CH<sub>3</sub>I 212 (1993) 124
- Szalay, P.G. and R.J. Bartlett, Multi-reference averaged quadratic coupled-cluster method: a size-extensive modification of multi-reference CI 214 (1993) 481
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- Tachikawa, E., see Y. Fujitani 214 (1993) 301
- Tachikawa, H., Reaction mechanism of the radical isomerization from  $\text{CH}_3\text{O}$  to  $\text{CH}_2\text{OH}$  in frozen methanol. An ab initio MO and RRKM study 212 (1993) 27
- Tachiya, M., see A.V. Barzykin 216 (1993) 575
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- Tahara, T. and H. Hamaguchi, Transient Raman spectra and structure of the "twisted" excited singlet state of tetraphenylethylene 217 (1994) 369
- Tahara, T., see T. Tsukuda 218 (1994) 1
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- Taiti, C., P. Foggi, G.F. Signorini and V. Schettino, Vibrational relaxation of a  $\text{MnO}_4^-$  impurity mode in  $\text{KClO}_4$  crystal 212 (1993) 283
- Takada, T., see M. Tomonari 215 (1993) 45
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- Takagi, N., J. Yoshinobu and M. Kawai, Direct observation of isothermal adsorption and desorption processes of CO on the Ni(100) surface 215 (1993) 120
- Takahashi, A., H.X. Wang and S. Mukamel, Collective charge density fluctuations and nonlinear optical response of  $\text{C}_{60}$  216 (1993) 394
- Takahashi, H., see J. Watanabe 213 (1993) 351
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- Takaoka, T., Y. Yasui, M. Sawada, T. Aruga and M. Nishijima, Coadsorption of CO and  $\text{C}_2\text{H}_4$  on Pd(110). Formation of a (3×2) mixed structure 215 (1993) 523
- Takasu, R., Y. Fujiwara and M. Itoh, No excited state proton transfer takes place in jet-cooled methanol clusters of 3-hydroxyflavone 217 (1994) 478
- Takayanagi, M., see T. Gejo 218 (1994) 343
- Takeda, J., T. Tayu, S. Kurita, Y. Yokoyama, Y. Kurita, T. Kuga and M. Matsuoka, Radiative and non-radiative decay processes of the excited state of the colored form of photochromic furylfulgide 220 (1994) 443
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- Tamai, N., C.F. Porter and H. Masuhara, Femtosecond transient absorption spectroscopy of a single perylene microcrystal under a microscope 211 (1993) 364
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- Tang, J., Superexchange electron-transfer reactions in a three-component system. The spin-boson model for photosynthesis 217 (1994) 55
- Tang, J., M.C. Thurnauer and J.R. Norris, Electron spin echo envelope modulation due to exchange and dipolar interactions in a spin-correlated radical pair 219 (1994) 283
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- Tani, T., see V.F. Kamalov 220 (1994) 257
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- Tchougreeff, A.L., The origin of cooperativity in high-spin-low-spin transitions in molecular crystals 214 (1993) 627
- Teixeira-Dias, J.J.C., see R.D. Gordon 211 (1993) 392
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- Ten-no, S., An efficient algorithm for electron repulsion integrals over contracted Gaussian-type functions 211 (1993) 259
- Ten-no, S., F. Hirata and S. Kato, A hybrid approach for the solvent effect on the electronic structure of a solute based on the RISM and Hartree-Fock equations 214 (1993) 391
- Terazima, M. and N. Hirota, Time-resolved two-step excitation thermal grating method. Measurement of the quantum yield of energy transfer from a higher excited triplet state 214 (1993) 541
- Terazima, M., Measurement of translational diffusion of a photochemically stable molecule by the transient grating method. Hematoporphyrin in acetone 218 (1994) 574
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- Thelen, M.-A., P. Felder and J.R. Huber, The photofragmentation of methyl hydroperoxide  $\text{CH}_3\text{OOH}$  at 193 and 248 nm in a cold molecular beam 213 (1993) 275
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- Tipikin, D.S., Ya.S. Lebedev, O.G. Poluektov and J. Schmidt, ESE-detected EPR of triplet radical pairs produced by mechano-chemical treatment of 2,6-di-*t*-butylquinone diazide mixed with 3,5-di-*t*-butylpyrocatechon 215 (1993) 199
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- Tomer, J.L., M.C. Wall, B.P. Reid and J.I. Cline, Photofragmentation dynamics of 2-chloro-2-nitrosopropane. Scalar correlations of velocity and angular momentum 216 (1993) 286
- Tominaga, K., see R. Inaba 211 (1993) 183
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- Torre, R., I. Santa and R. Righini, Pre-transitional effects in the liquid-plastic phase transition of *p*-terphenyl 212 (1993) 90
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- Tossell, J.A., The relationship between the inner-shell electron energy-loss spectra and the  $^{29}\text{Si}$  NMR spectra of the chlorosilanes,  $\text{SiH}_x\text{Cl}_{4-x}$ . An interpretation of the trend in NMR shieldings 219 (1994) 65
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- Tran-Thi, T.-H., T. Fournier, A. De Cian, D. Chabach, R. Weiss, D. Houde, C. Pépin and L. Dao, Picosecond relaxation of charge transfer states in an asymmetric cerium double-decker sandwich compound 213 (1993) 139
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- Triebel, M.M., M.M. Totrov, G.E. Zorinyants and E.L. Frankevich, The use of the magnetic field effect for studying a chemiluminescent chemical reaction in aqueous solution. Reaction rate constants and lifetimes of intermediate molecules 214 (1993) 315
- Triebel, M.M., A.K. Morozov, M.M. Totrov, G.E. Zorinyants and E.L. Frankevich, Phase-on-frequency characteristics of the magnetic field effect for studying the mechanism of the branching chemiluminescent reaction of luminol 214 (1993) 321
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- Tse, J.S., B.M. Powell, V.F. Sears and Y.P. Handa, The lattice dynamics of clathrate hydrates. An incoherent inelastic neutron scattering study 215 (1993) 383
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- Tsukuda, T., M. Nagaminé, T. Tahara, T. Nagata and T. Kondow, Competitive electron capture in mixed clusters,  $\text{X}(\text{HCN})_m$  ( $\text{X} = \text{C}_2\text{H}_5\text{OH}$ ,  $\text{CO}_2$ ,  $\text{O}_2$ , and  $\text{SF}_6$ ) 218 (1994) 1

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- Uehara, H., K. Horiai, A. Kerim, Y. Ozaki and T. Konno, Infrared emission spectrum of NaBr 213 (1993) 101
- Uehara, H., K. Horiai, Y. Ozaki and T. Konno, Infrared emission spectrum of AlBr 214 (1993) 527
- Uehara, H., K. Horiai, Y. Ozaki and T. Konno, Infrared diode laser spectroscopy of high-temperature molecules using spectrum processing by Fourier transformation 215 (1993) 505
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- Vacek, J., K. Konvička and P. Hobza, A molecular dynamics study of the benzene...Ar<sub>2</sub> complex. Application of the nonempirical ab initio and empirical Lennard-Jones 6-12 potentials 220 (1994) 85
- Vachev, V.D., J.H. Frederick, B.A. Grishanin, V.N. Zadkov and N.I. Koroteev, Stilbene isomerization dynamics on multidimensional potential energy surface. Molecular dynamics simulation 215 (1993) 306
- Vahtras, O., J. Almlöf and M.W. Feyereisen, Integral approximations for LCAO-SCF calculations 213 (1993) 514
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- Valent, I. and L. Adamčíková, The clock behavior of the BrO<sub>3</sub><sup>-</sup>-SCN<sup>-</sup> reaction 216 (1993) 479
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- Van den Hoek, G., M. Jonker, D.H. Parker, C.A. Taatjes and S. Stolte, Double-resonance measurements of vibrational levels populated by infrared multiphoton excitation of CF<sub>3</sub>I in a molecular beam 215 (1993) 461
- Van der Auweraer, M., see S. Depaemelaere 215 (1993) 649
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- Van der Laan, H., C. De Caro, Th. Schmidt, R.W. Visschers, R. van Grondelle, G.J.S. Fowler, C.N. Hunter and S. Völker, Excited-state dynamics of mutated antenna complexes of purple bacteria studied by hole-burning 212 (1993) 569
- Van der Maarel, J.R.C., see T.W.N. Bieze 216 (1993) 56
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- Van Dijk, S.I., P.G. Wiering, R. van Staveren, H.J. van Ramesdonk, A.M. Brouwer and J.W. Verhoeven, Two-step photoinduced charge separation and unexpectedly fast one-step charge recombination in a linked donor<sub>2</sub>-donor<sub>1</sub>-acceptor system 214 (1993) 502
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- Van Zee, R.J., S. Li and W. Weltner Jr., Ground electronic states of ZrO<sup>+</sup>, HfO<sup>+</sup>, and Nb<sub>2</sub><sup>+</sup>. ESR spectra of the matrix-isolated ions 217 (1994) 381
- Vauthey, E., D. Pilloud, E. Haselbach, P. Suppan and P. Jacques, The reliability of free ion yield in photoinduced electron transfer reactions. The model system 9,10-dicyanoanthracene/biphenyl in acetonitrile 215 (1993) 264
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- Von Helden, G., N.G. Gotts and M.T. Bowers,  $C_7^+$  is cyclic: experimental evidence 212 (1993) 241
- Von Helden, G., W.E. Palke and M.T. Bowers, The lowest energy structures of  $C_7^+$ ,  $C_7$  and  $C_7^-$ . An ab initio study 212 (1993) 247
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- Wallington, T.J., M.D. Hurley and W.F. Schneider, Kinetic study of the reaction  $\text{CF}_3\text{O} + \text{O}_3 \rightarrow \text{CF}_3\text{O}_2 + \text{O}_2$  213 (1993) 442
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- Wang, J. and V.H. Smith Jr., Evaluation of electron pair densities and their Laplacians in atomic systems 220 (1994) 331
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- Wang, K., V. McKoy and H. Rudolph, Rotationally resolved photoelectron spectra in (2+1) resonance-enhanced multiphoton ionization of NO via the  $\text{C } ^2\Pi$  Rydberg state 217 (1994) 490
- Wang, K., M.-T. Lee, V. McKoy, R.T. Wiedmann and M.G. White, Rotationally resolved threshold photoelectron spectroscopy of  $\text{H}_2\text{O}$  and  $\text{H}_2\text{S}$  219 (1994) 397
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- Wang, X.-D., T. Hashizume, Q. Xue, H. Shinohara, Y. Saito, Y. Nishina and T. Sakurai, Geometry of metallofullerenes adsorbed on the Si(100)2×1 surface studied by scanning tunneling microscopy 216 (1993) 409
- Wang, X.Q., C.Z. Wang, B.L. Zhang and K.M. Ho, First-principles study of C<sub>96</sub> fullerene isomers 214 (1993) 193
- Wang, X.Q., C.Z. Wang, B.L. Zhang and K.M. Ho, Electronic structures of C<sub>82</sub> fullerene isomers 217 (1994) 199
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- Wang, Y., C.A. Woodward and W.A. Chupka, Ionic state preparation of O<sub>2</sub><sup>+</sup> via the 3dδ<sup>1,3</sup>Φ<sub>g</sub> Rydberg states of O<sub>2</sub> 214 (1993) 290
- Wang, Y., J.M. Holden, X. Bi and P.C. Eklund, Thermal decomposition of polymeric C<sub>60</sub> 217 (1994) 413
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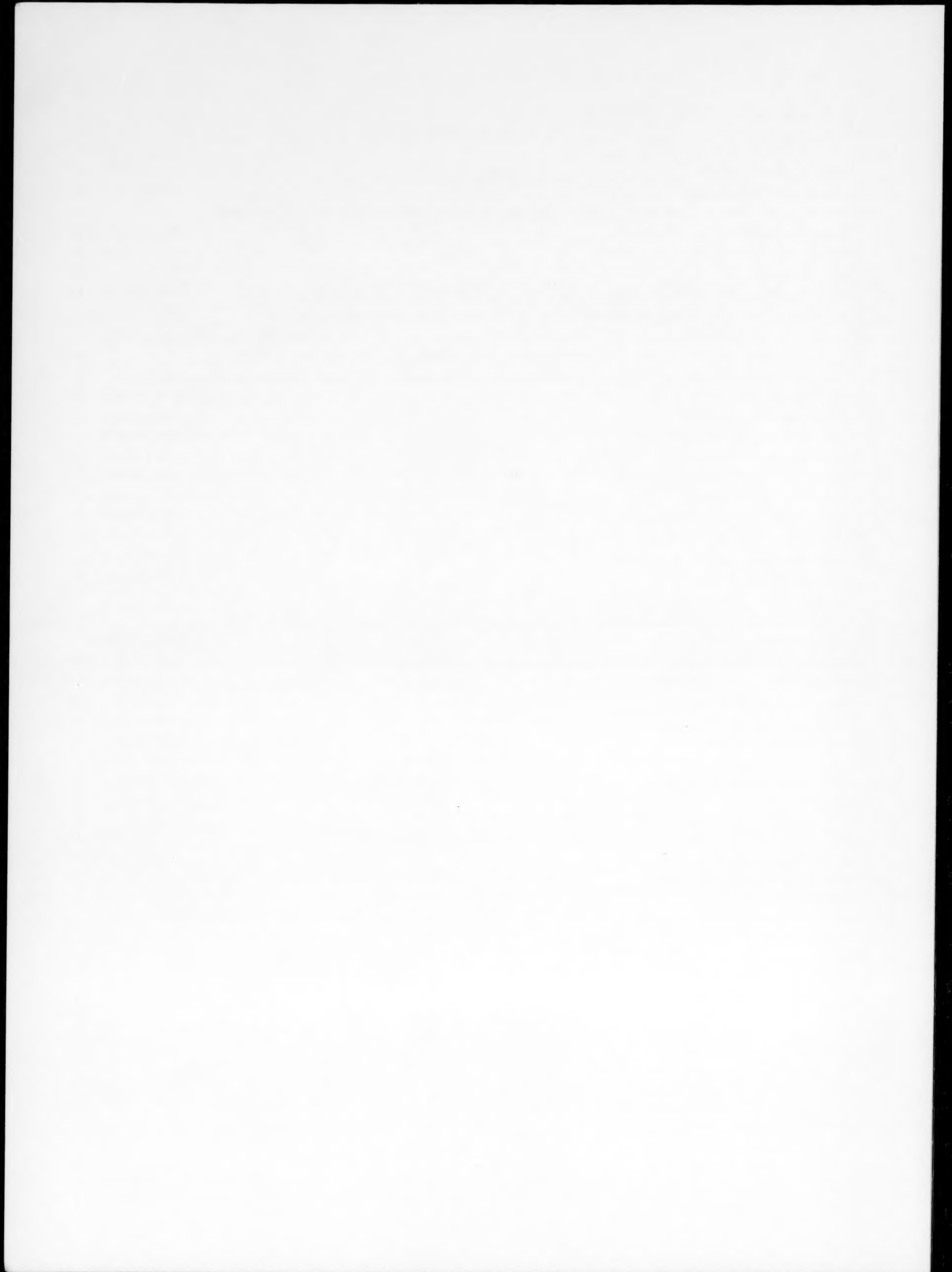
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# Mössbauer Studies of Surface Layers

By G.N. Belozerski

Studies in Physical and Theoretical Chemistry Volume 81

Mössbauer spectroscopy has evolved as one of the few methods available for investigation of solids differing in depth by several orders of magnitude. This recent development has made the problems of surface investigation and the study of separate layers amenable to investigation. The parameters of the hyperfine interaction derived from the Mössbauer spectra provide valuable information on the chemical bond character and on magnetic properties of surface layers as well as on the change of the properties with the depth from the outermost surface layer. It is possible to carry out quantitative phase analysis and to use the technique to study different transformations in the solid which result from external effects under a wide range of temperatures and pressures.

This book is one of the first attempts at a consistent presentation of theoretical and practical problems of the use of Mössbauer spectroscopy to study solid surfaces, its applications, and development. The applications include: surface studies with hyperfine probes in the following fields: oxidation and corrosion of metals and alloys; passivating and protective coatings; physics of metals; annealing and quenching, mechanical and chemical treatment, ion implantation and laser treatment; texture of near-surface layers.

Mössbauer spectroscopy is one of the best methods for *in situ* characterization of solid/solid and solid/solution interfaces. It lends itself to *in situ* studies of surfaces under various coatings and processes, surface magnetism and the effect of the gas phase on the properties of the surface layers and the structure and magnetic properties of epitaxially grown monolayers on the surface of oriented single crystals.

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# Inorganic Polymeric Glasses

By **R.C. Ropp**, Warren, NJ, USA

Studies in Inorganic Chemistry Volume 15

The author describes a novel method of preparing hydrolysis-stable non-silicate glasses which is based on experimental work accomplished over the past twenty years. As such, the method is the beginning of a new approach to glass-making by the use of a molecularly-polymerizable precursor.

The book elucidates the technical details required to produce such molecularly-polymerized glasses from carefully prepared inorganic molecular monomers. Essentially, only silicate-based glasses have been known to be stable, whereas non-silicate glasses could not be attributed with such properties. Such glasses have, therefore, not found widespread usage in industry. The new phosphate glasses described here exhibit stabilities superior to many of the silicate glasses.

Researchers in glass and glass properties will find this volume extremely useful and those involved in organic polymers will be intrigued by the similarities and disparities of the two systems.

## **Contents: 1. Introduction to Silicate Glass Technology.**

Glass and Antiquity. The Glassy or Vitreous State. Glass Formers and Glass Compositions. The Manufacture of Silicate-Based Glasses. Forming and Finishing Operations. Thermal Processing and Properties of Silicate Glasses. Inherent Properties of Glass. Silicate Glass Products Currently being Manufactured.

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# Dynamics of Excited Molecules

Edited by Kozo Kuchitsu

Studies in Physical and Theoretical Chemistry Volume 82

The physical and chemical properties of the molecular species reviewed in this book, and sometimes the species themselves, had been postulated or predicted but their exact details remained essentially unexplored for decades. The recent advances in chemical physics (such as laser spectroscopy and quantum-theoretical calculations) have provided techniques for their unambiguous identification. Accurate data on their structures and dynamics are now available. Such information is indispensable for detailed discussion on the various properties of molecules and the mechanisms of intermolecular interactions and chemical interactions.

Information on the dynamics of excited molecules constitutes a firm basis of modern chemistry and physics. Moreover, it is of paramount importance in various fields of basic and applied sciences where chemical reactions play important roles: atomic and molecular physics, atmospheric and environmental science, space science, materials science, and biology.

This book contains 13 review articles on

(1) the techniques for production and identification of excited molecules in the gas phase, condensed phases, and intermediate phases (intermolecular complexes and atomic or molecular microclusters)  
(2) their structures and dynamics (internal reactions) observed

mainly by spectroscopic experiments

(3) their important roles in chemical processes. The target chemical species range from diatomics to relatively complicated aromatics in a variety of electronic and vibrational excited states, many of them being nonrigid or short-lived molecules, radicals, and positive or negative ions.

## Contents:

1. Dynamics of excited molecules. An introduction (K. Kuchitsu, S. Tsuchiya).
  2. Infrared diode laser and microwave kinetic spectroscopy (H. Kanamori *et al.*).
  3. Free jet infrared spectroscopy of weakly bound complexes (M. Takami *et al.*).
  4. Large-amplitude motions of aromatic molecules as studied by supersonic jet spectroscopy (M. Ito).
  5. Decay processes of inner-shell photoexcited molecules (Y. Sato)
  6. Dynamics of superexcited molecules (Y. Hatano).
  7. Vibrational dynamics in highly excited polyatomic molecules (K. Yamanouchi, S. Tsuchiya).
  8. Dynamics of ion-molecule reactions (I. Koyano).
  9. Multiphoton ionization spectroscopy (H. Sato).
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  11. Gas-phase cluster ions: stability, structure and solvation (K. Hiraoka, S. Yamabe).
  12. Chemistry of gas-phase microclusters (K. Kaya, T. Kondow).
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# Physico-Chemical Properties of Selected Anionic, Cationic and Nonionic Surfactants

by N.M. van Os, J.R. Haak and L.A.M. Rupert

The number of physico-chemical investigations of surfactants in solution, whether aqueous or nonaqueous, has dramatically increased in recent years. However, literature reports on surfactants in solutions are scattered over a plethora of scientific journals and books which differ widely in scope and readership. Such data are often difficult to retrieve because there have been no systematic compilations, with the exception of those for CMCs and for micelle aggregation numbers.

The present compilation meets that need by covering, as completely as possible, the physico-chemical properties of selected series of homologous surfactants. These surfactants are in most cases isomerically pure, are well-known, and have been used in numerous academic and industrial studies. The properties include aggregation number, cloud point, CMC,  $^{13}\text{C}$ -NMR, correlation length, counterion binding, density, enthalpy of micelle formation, entropy of micelle formation, Gibbs' free energy of micelle formation, head group area,  $^1\text{H}$ -NMR, hydration number, Krafft temperature, melting point, micelle radius, microscopic viscosity, miscibility curve, partial molar volume,

phase inversion temperature, refractive index, self-diffusion coefficient, surface tension, and upper critical temperature. The book also contains two- and three-component phase diagrams of many nonionic surfactants.

The solvent is water in most cases; however, some data refer to properties in  $\text{D}_2\text{O}$ , electrolyte solutions, and nonaqueous solvents. The variables are temperature and concentration. Where possible, the method of measurement is given. Data on the purity of the compounds and the accuracy of the measurement methods are not included, as these can easily be found in the original sources, which mostly date from the period 1970-1991 and are given at the end of each chapter. The Index section contains a compound index, a property index, a symbol index and a cross index which facilitate easy access to the data.



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**Part III: Nonionic Surfactants.** Alkylpolyoxyethylene Glycol Ethers. Alkylphenol(ethylene oxide) Ethers.  
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